

chain nodes :

16 17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

ring/chain nodes :

14 15

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

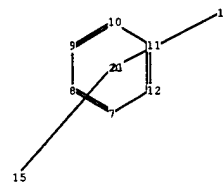
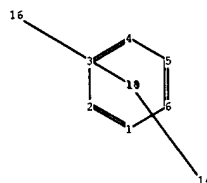
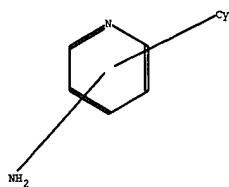
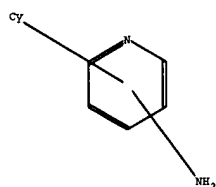
isolated ring systems :

containing 1 : 7 :

G1:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:CLASS
19:CLASS 20:CLASS 21:CLASS



chain nodes :

16 17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

ring/chain nodes :

14 15

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

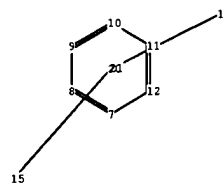
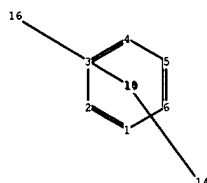
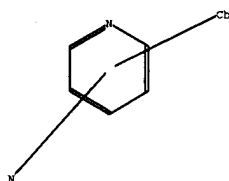
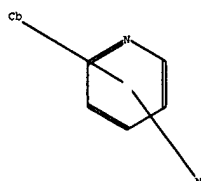
isolated ring systems :

containing 1 : 7 :

G1:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:CLASS
19:CLASS 20:CLASS 21:CLASS



chain nodes :

16 17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

ring/chain nodes :

14 15

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

isolated ring systems :

containing 1 : 7 :

G1:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:CLASS
19:CLASS 20:CLASS 21:CLASS

09/893,680

=> d his

(FILE 'HOME' ENTERED AT 12:09:57 ON 11 SEP 2002)

FILE 'REGISTRY' ENTERED AT 12:10:03 ON 11 SEP 2002

L1 STRUCTURE UPLOADED
L2 QUE L1
L3 0 S L2
L4 373 S L2 SSS FUL

FILE 'CAPLUS' ENTERED AT 12:11:24 ON 11 SEP 2002

L5 102 S L4
DEL A08952817/A
DEL A09113905/A
DEL A09446736/L
DEL B09113905/A

FILE 'REGISTRY' ENTERED AT 12:13:27 ON 11 SEP 2002

L6 STRUCTURE UPLOADED
L7 QUE L6
L8 53 S L7 SUB=L4 FUL
L9 320 S L4 NOT L8

FILE 'CAPLUS' ENTERED AT 12:20:39 ON 11 SEP 2002

L10 85 S L9
L11 33 S L10 AND PATENT/DT
L12 52 S L10 NOT L11
L13 2 S L12 AND 2002/SO

FILE 'REGISTRY' ENTERED AT 12:22:57 ON 11 SEP 2002

L14 STRUCTURE UPLOADED
L15 QUE L14
L16 3 S L15 SUB=L9 SAM
L17 84 S L15 SUB=L9 FUL
L18 236 S L9 NOT L17

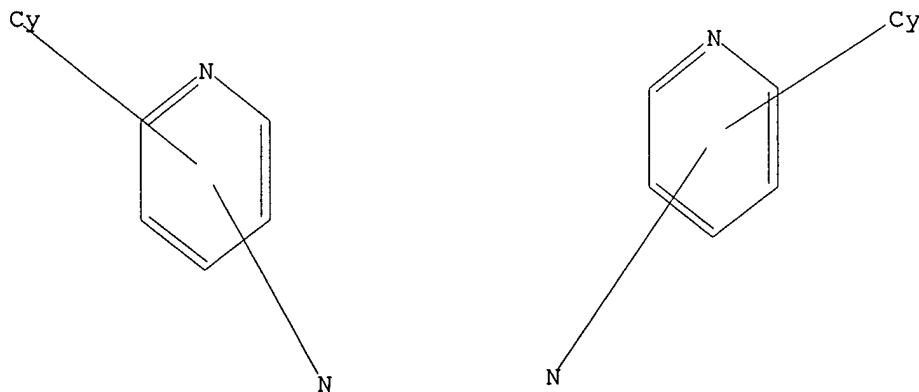
FILE 'CAPLUS' ENTERED AT 12:26:17 ON 11 SEP 2002

L19 21 S L17

=> d l2

L2 HAS NO ANSWERS

L1 STR

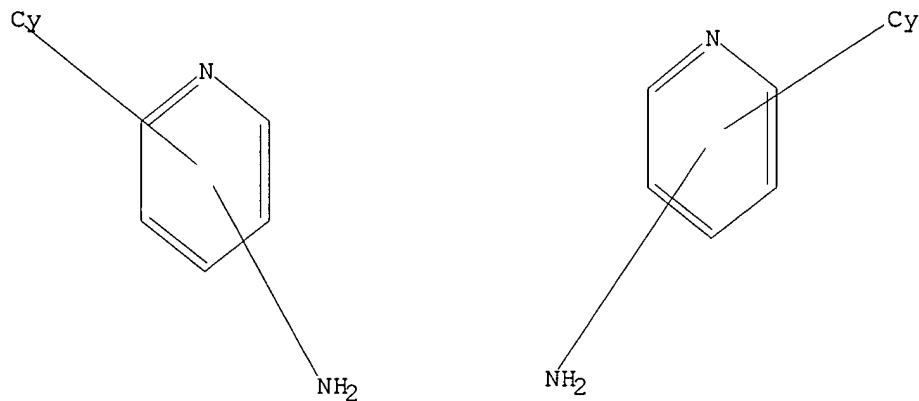


G1 C,N

09/893,680

Structure attributes must be viewed using STN Express query preparation.
L2 QUE ABB=ON PLU=ON L1

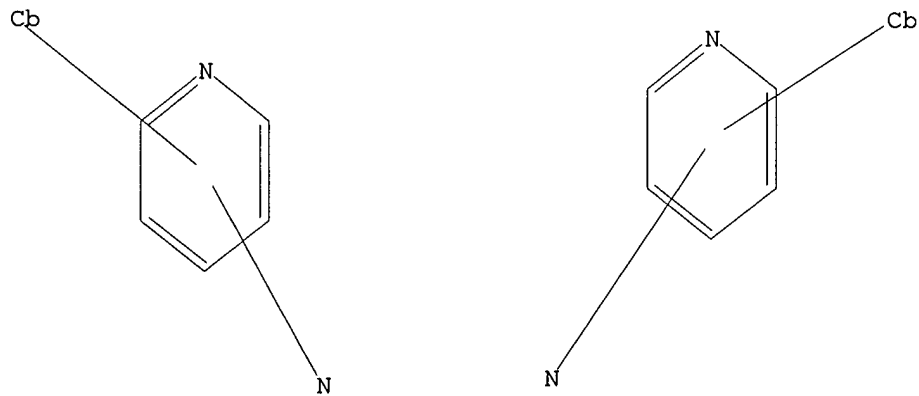
=> d 17
L7 HAS NO ANSWERS
L6 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.
L7 QUE ABB=ON PLU=ON L6

=> d 115
L15 HAS NO ANSWERS
L14 STR



G1 C,N

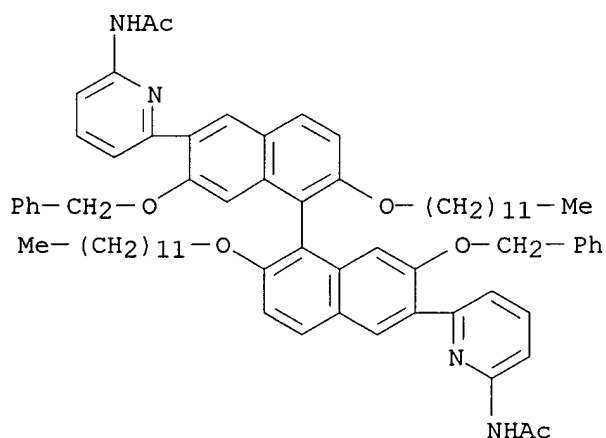
Structure attributes must be viewed using STN Express query preparation.
L15 QUE ABB=ON PLU=ON L14

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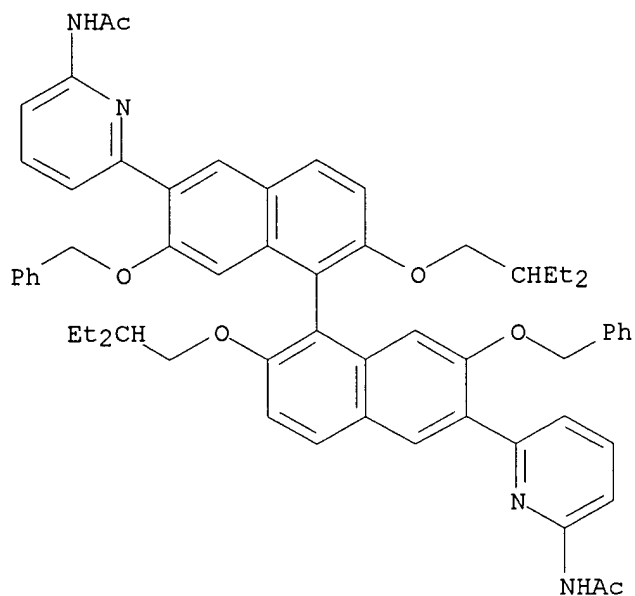
=> d bib abs hitstr 119 1-21

09/893,680

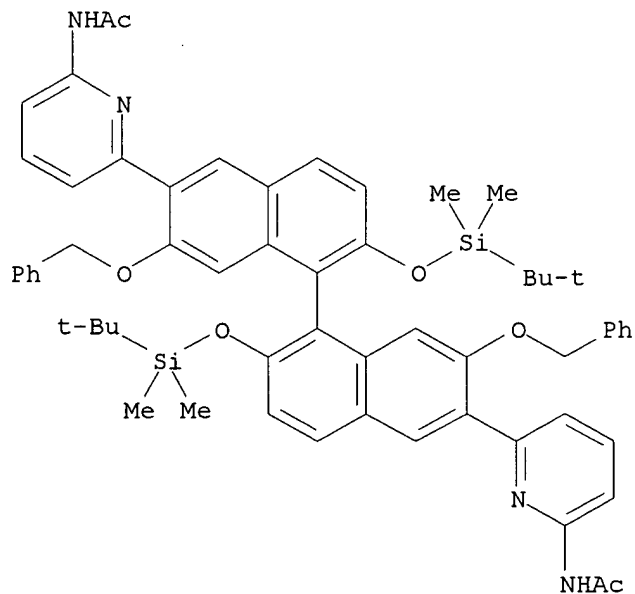
~~LA~~ 9 ANSWER 1 OF 21 CAPLUS COPYRIGHT 2002 ACS
AN 2000:543469 CAPLUS
DN 133:266471
TI Conformational Analysis in Solution of C2-Symmetric 1,1'-Binaphthyl
Derivatives by Circular Dichroism Spectroscopy and Cholesteric Induction
in Nematic Mesophases
AU Proni, Gloria; Spada, Gian Piero; Lustenberger, Philipp; Welty, Roger;
Diederich, Francois
CS Dipartimento di Chimica Organica A. Mangini, Universita di Bologna,
Bologna, I-40127, Italy
SO Journal of Organic Chemistry (2000), 65(18), 5522-5527
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
AB The twisting ability of a series of 1,1'-binaphthalene compds. used as
dopants in nematic solvents has been related to the dihedral angle .theta.
between the two naphthalene moieties. While in the case of the more
flexible compds. the sign and value of the helical twisting power is
affected by several structural features that prevent a simple assignment
of the conformation, in the presence of a covalent bridge that restricts
the rotation around the C(1)-C(1') bond a reliable est. of the
conformational helicity could be obtained. This technique is
complementary to CD spectroscopy that, for the investigated mols.,
presents the same exciton patterns irresp. of the actual .theta. value.
IT 171976-27-5 205940-00-7 205940-01-8
205940-05-2 205940-06-3
RL: PRP (Properties)
(conformational anal. in soln. of C2-sym. binaphthyl derivs. by CD
spectroscopy and cholesteric induction in nematic mesophases)
RN 171976-27-5 CAPLUS
CN Acetamide, N,N'-[[(1R)-2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy) [1,1'-
binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis- (9CI) (CA INDEX NAME)



RN 205940-00-7 CAPLUS
CN Acetamide, N,N'-[[2,2'-bis(2-ethylbutoxy)-7,7'-bis(phenylmethoxy) [1,1'-
binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (R)- (9CI) (CA INDEX
NAME)

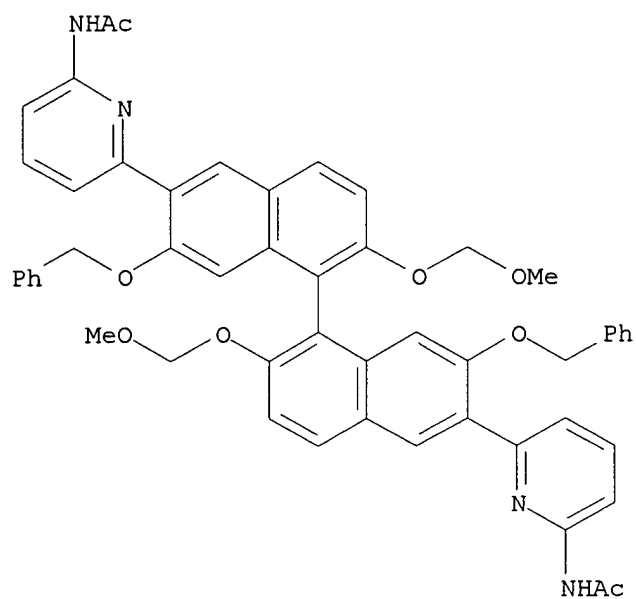


RN 205940-01-8 CAPLUS
 CN Acetamide, N,N'-[[2,2'-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7,7'-bis(phenylmethoxy) [1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (R)- (9CI) (CA INDEX NAME)

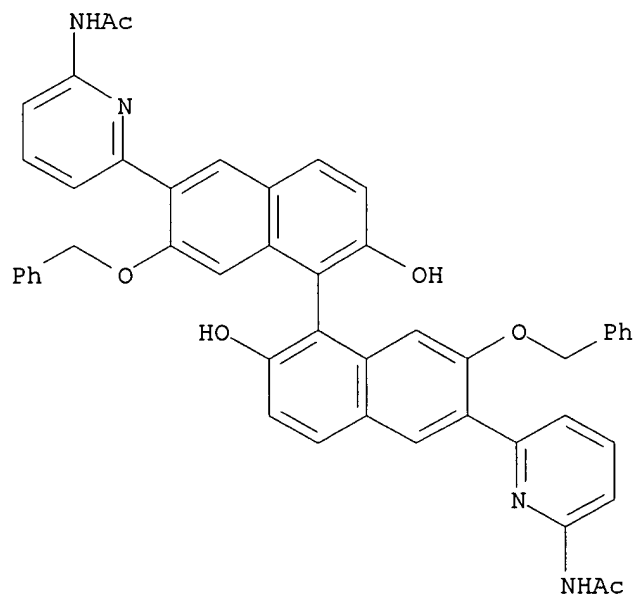


RN 205940-05-2 CAPLUS
 CN Acetamide, N,N'-[[2,2'-bis(methoxymethoxy)-7,7'-bis(phenylmethoxy) [1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (R)- (9CI) (CA INDEX NAME)

09/893,680



RN 205940-06-3 CAPLUS
CN Acetamide, N,N'-[[2,2'-dihydroxy-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (R)- (9CI) (CA INDEX NAME)



RE.CNT 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~LN~~ 9 ANSWER 2 OF 21 CAPLUS COPYRIGHT 2002 ACS
~~AN~~ 2000:125442 CAPLUS
DN 132:264946
TI Cleft-type diamidinium receptors for dicarboxylate binding in protic solvents
AU Sebo, Lubomir; Schweizer, Bernd; Diederich, Francois
CS Laboratorium fur Organische Chemie der Eidgenossischen Technischen Hochschule, Laboratorium fur Organische Chemie der Eidgenossischen Technischen Hochschule, ETH-Zentrum, Zurich, CH-8092, Switz.
SO Helvetica Chimica Acta (2000), 83(1), 80-92
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta
DT Journal
LA English
AB A series of potential cleft-type receptors for dicarboxylate substrates were prep'd. by attachment of two phenylamidinium ions to either naphthalene or 1,1'-binaphthalene scaffolds. Their synthesis involved the Pd0-catalyzed cross-coupling of aryl nitriles to the central scaffold, followed by transformation of the nitrile into amidinium groups using the Garigipati reaction. The 1,1'-binaphthalene deriv. with phenylamidinium residues attached to the 6,6'-positions(I) in the major groove is a highly efficient receptor for dicarboxylate guests, such as glutarate and isophthalates, even in competing protic solvents such as CD3OD. The van't Hoff anal. of variable-temp. 1H-NMR (VT-NMR) titrns. and isothermal microcalorimetry revealed that complexation in MeOH is strongly entropically driven with an unfavorable enthalpic change, which partially compensates the entropic gain. These thermodyn. quantities are best explained by a particularly favorable solvation of the binding partners in the unbound state and the release of the MeOH mols., which solvate the free ions into the bulk upon complexation. Receptor I binds flexible glutarate and rigid isophthalates with similar assocn. strength. This lack in response to guest preorganization and reduced guest selectivity is explained with the non-directionality of the coulombic charge-charge interactions in the complexes.

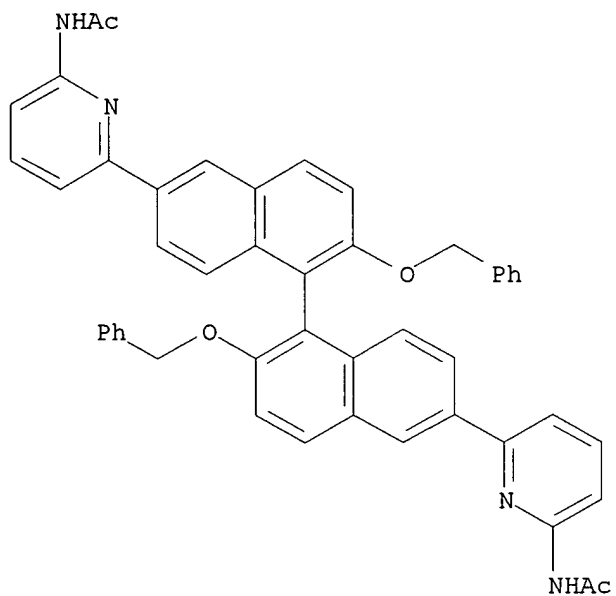
IT **147580-15-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of cleft-type diamidinium receptors for dicarboxylate binding)

RN 147580-15-2 CAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-(dodecyloxy)-, comp'd. with
N,N'-[[2,2'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147580-10-7
CMF C48 H38 N4 O4

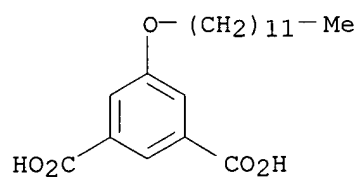
09/893,680



CM 2

CRN 147580-08-3

CMF C20 H30 O5



RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~L19~~ ANSWER 3 OF 21 CAPLUS COPYRIGHT 2002 ACS

~~AN~~ 1999:49664 CAPLUS

~~DN~~ 130:182446

~~TI~~ Negative cooperativity in the molecular recognition of excitatory amino-acid derivatives by synthetic allosteric 1,1'-binaphthalene receptors

~~AU~~ Lustenberger, Philipp; Welte, Roger; Diederich, Francois

~~CS~~ Laboratorium Organische Chemie, Eidgenoessische Technische Hochschule Zurich, Zurich, CH-8092, Switz.

~~SO~~ Helvetica Chimica Acta (1998), 81(12), 2190-2200

CODEN: HCACAV; ISSN: 0018-019X

~~PB~~ Verlag Helvetica Chimica Acta AG

~~DT~~ Journal

~~LA~~ English

~~AB~~ Optically active allosteric receptors were synthesized for the mol. recognition of N-(benzyloxy)carbonyl (N-Cbz)-protected excitatory aspartic acid (Asp) and glutamic acid (Glu). These macrocyclic structures consist of 2 1,1'-binaphthalene moieties connected by 2 but-2-yne-1,4-diyl or 1,4-xylylene bridges between the O-atoms in the minor grooves. Each 1,1'-binaphthalene moiety contains 2 2-acetamidopyridin-6-yl [CONH(py)] H-bonding sites in the major groove to bind excitatory amino acids via 2 CO2H...CONH(py) H-bonding arrays and addnl. secondary electrostatic interactions. The formation of stable complexes with 1:2 host-guest stoichiometry was proven by the evaluation of fluorescence binding titrns. using a multiple-wavelength nonlinear least-squares curve-fitting procedure, Job plot anal., and solubilization expts. Complexation of the first excitatory amino-acid guest at binding site 1 reduces the affinity for the second guest at binding site 2. As measures for the neg. cooperativity between the 2 sides, the ratios of the assocn. consts. for the first and second binding events, $\{K_a(1:1)/K_a(1:2)\}_{corr.}$ (cor. for the statistical preference of the 1:1 complex formation), adopt values between 1.4 and 2.4, and the Hill coeffs. n_H varied between 0.49 and 0.59.

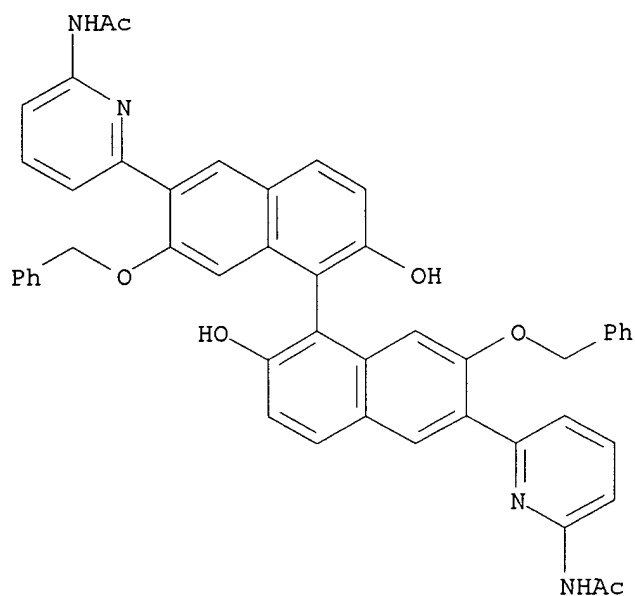
~~IT~~ 205940-06-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of butynediyl- and xylylene-bridged allosteric binaphthalene receptors)

~~RN~~ 205940-06-3 CAPLUS

~~CN~~ Acetamide, N,N'-[[2,2'-dihydroxy-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (R)- (9CI) (CA INDEX NAME)



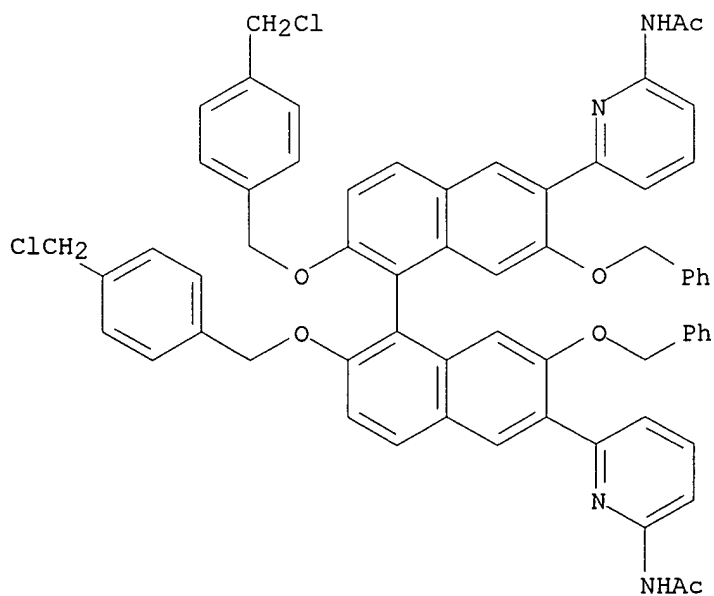
IT 220580-47-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of butynediyl- and xylylene-bridged allosteric binaphthalene receptors)

RN 220580-47-2 CAPLUS

CN Acetamide, N,N'-[[[(1R)-2,2'-bis[[4-(chloromethyl)phenyl]methoxy]-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-(9CI) (CA INDEX NAME)



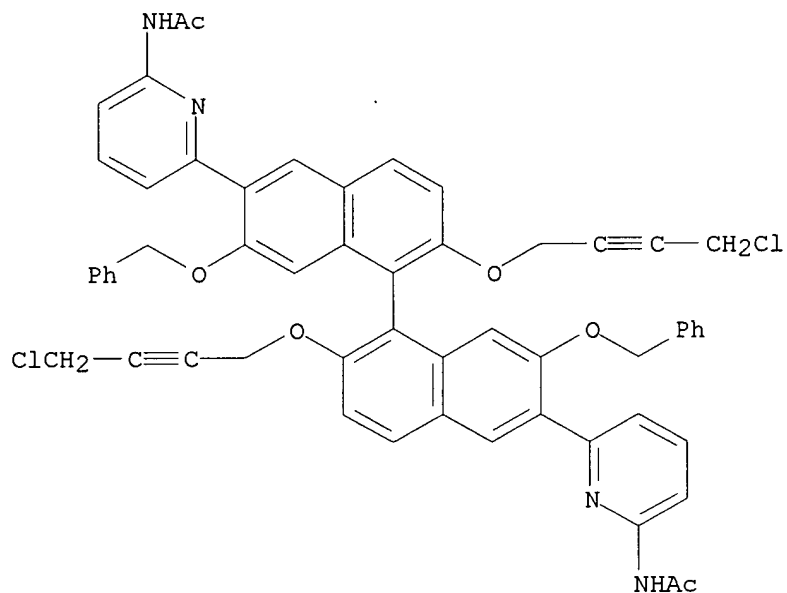
09/893,680

IT 220580-43-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of butynediyl- and xylylene-bridged allosteric binaphthalene
receptors)

RN 220580-43-8 CAPLUS

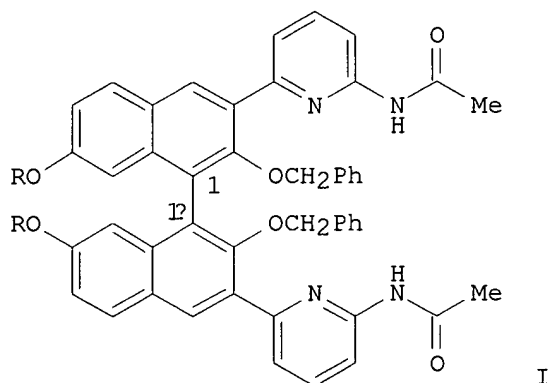
CN Acetamide, N,N'-[[(1R)-2,2'-bis[(4-chloro-2-butynyl)oxy]-7,7'-
bis(phenylmethoxy) [1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-
(9CI) (CA INDEX NAME)



RE.CNT 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

09/893,680

119 ANSWER 4 OF 21 CAPLUS COPYRIGHT 2002 ACS
AN 1998:180011 CAPLUS
DN 128:295007
TI Geometrical optimization of 1,1'-binaphthalene receptors for
enantioselective molecular recognition of excitatory amino acid
derivatives
AU Lustenberger, Philipp; Martinborough, Esther; Denti, Tiziana Mordasini;
Diederich, Francois
CS Laboratorium fur Organische Chemie, Zurich, CH-8092, Switz.
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic
Chemistry (1998), (4), 747-762
CODEN: JCPKBH; ISSN: 0300-9580
PB Royal Society of Chemistry
DT Journal; General Review
LA English
GI



AB A series of optically active 1,1'-binaphthalene-derived receptors I [R = Me(CH₂)₁₁, Et₂CHCH₂, Me₃CSiMe₂, 1-adamantylmethyl; R-R = CH₂, CH₂CH₂N+(Me₂)CH₂CH₂, CH₂CH₂N(CO₂Et)CH₂CH₂, CH₂CH₂NMeCH₂CH₂, CH₂C.tplbond.CCH₂, CH₂-m-C₆H₄CH₂] with (pyridine-2,6-diyl)acetamide hydrogen bonding sites in the 6,6'-positions has been prepd. for the enantioselective complexation of the protected excitatory amino acids Cbz-Asp-OH (Cbz = benzyloxycarbonyl) and Cbz-Glu-OH via two CO₂H-CONH(py) hydrogen bonding arrays and addnl. secondary bonding interactions. The conformational homogeneity of the receptors is enhanced by locking the dihedral angle .theta. about the chirality axis through the 1,1'-binaphthalene C(1)-C(1') bond either by bridging the 2,2'-positions or by attaching bulky substituents to these centers. Computer modeling has shown that bridging is more efficient in locking this dihedral angle than the introduction of bulky substituents, and these predictions have been confirmed by 1H NMR binding studies in CDCl₃ and in CDCl₃-CD₃OD (99.8:0.02). Plots of the enantioselectivity .DELTA.(.DELTA.G.degree.) (difference in stability between diastereoisomeric complexes) in the recognition by the bridged receptors as a function of the enforced dihedral angle .theta. are peak-shaped, and the highest values have been measured in CDCl₃ (300K) for the complexation of the enantiomers of Cbz-Asp-OH [.DELTA.(.DELTA.G.degree.) = 6.9 kJ mol⁻¹] and Cbz-Glu-OH

[Δ .(Δ .G .degree.) = 5.2 kJ mol⁻¹] by (R)-I (2R = CH₂CH₂NMeCH₂CH₂) (θ = 86 \pm 4.degree.). The more stable diastereoisomeric complexes are highly structured, and tight host-guest bonding has been confirmed by the observation of up to five intermol. NOEs. Enforcing the conformational homogeneity by bridging represents a new general principle for improving the chiral recognition potential of 1,1'-binaphthalene receptors. These data are preceded by a review describing the author's earlier work using helicene, spiro[bifluorene], and related binaphthyl-based receptors.

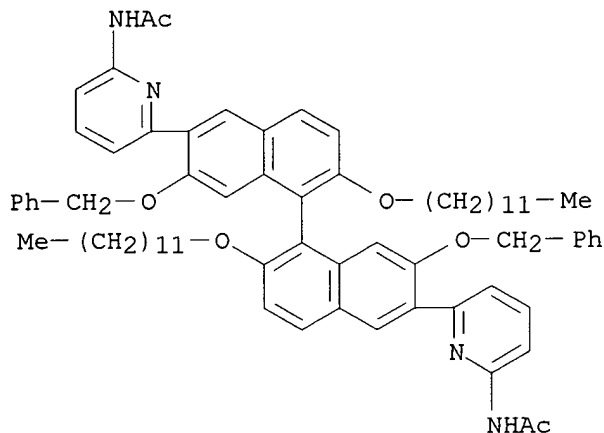
IT 171976-27-5

RL: PRP (Properties)

(prepn. and enantioselective excitatory amino acid recognition of bis(pyridinediylacetamide)binaphthalene receptors)

RN 171976-27-5 CAPLUS

CN Acetamide, N,N'-[[(1R)-2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy) [1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis- (9CI) (CA INDEX NAME)

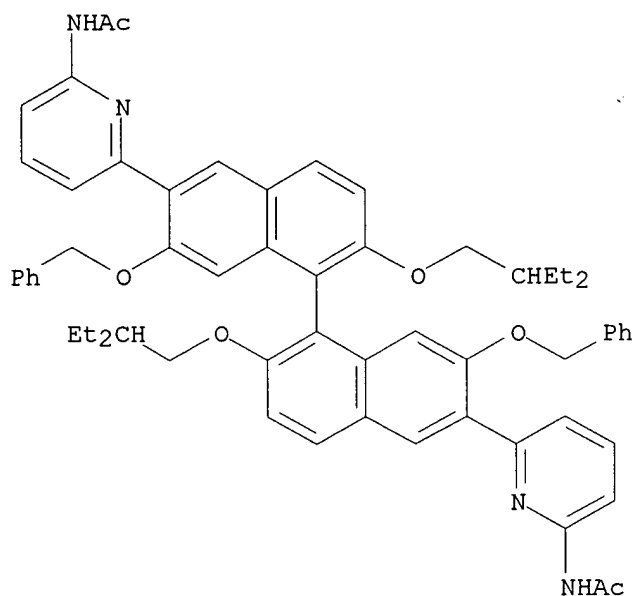


IT 205940-00-7P 205940-01-8P 205940-02-9P

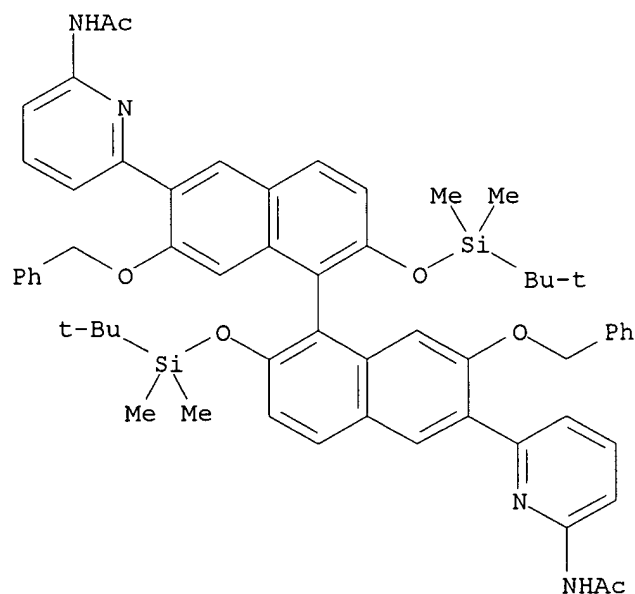
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and enantioselective excitatory amino acid recognition of bis(pyridinediylacetamide)binaphthalene receptors)

RN 205940-00-7 CAPLUS

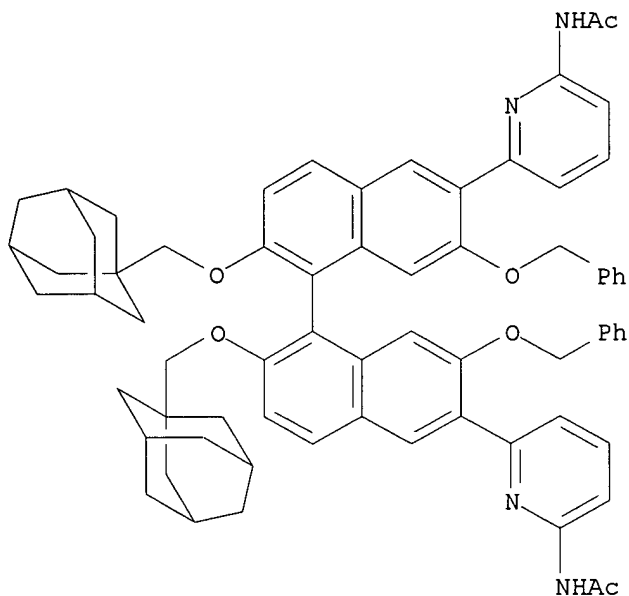
CN Acetamide, N,N'-[[2,2'-bis(2-ethylbutoxy)-7,7'-bis(phenylmethoxy) [1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (R)- (9CI) (CA INDEX NAME)



RN 205940-01-8 CAPLUS
 CN Acetamide, N,N'-[[2,2'-bis[[1,1-dimethylethyl]dimethylsilyl]oxy]-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (R)- (9CI) (CA INDEX NAME)



RN 205940-02-9 CAPLUS
 CN Acetamide, N,N'-[[7,7'-bis(phenylmethoxy)-2,2'-bis(tricyclo[3.3.1.1.3,7]dec-1-ylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (R)- (9CI) (CA INDEX NAME)



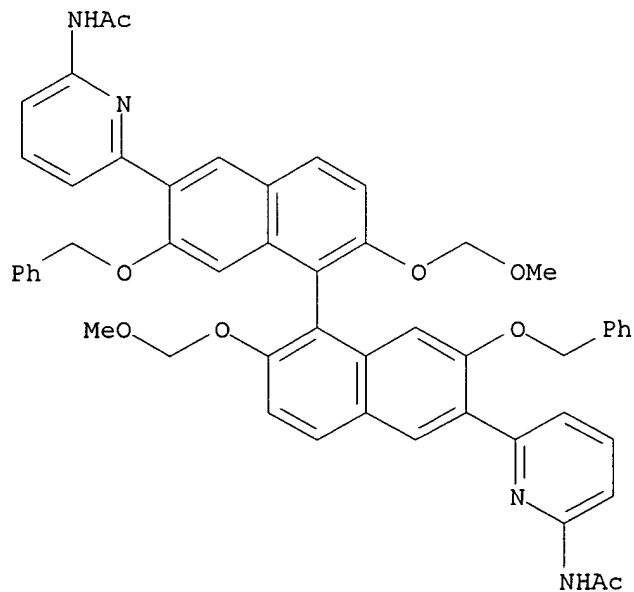
IT 205940-05-2P 205940-06-3P 205940-13-2P
205940-14-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(prepn. and enantioselective excitatory amino acid recognition of
bis(pyridinediylacetamide)binaphthalene receptors)

RN 205940-05-2 CAPLUS

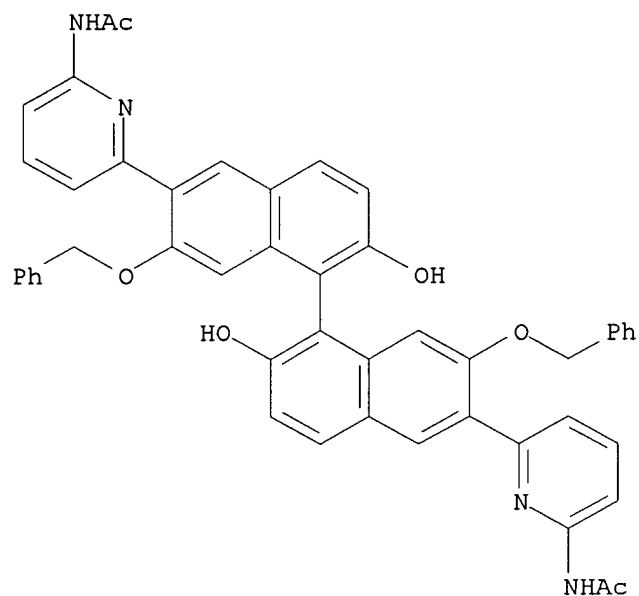
CN Acetamide, N,N'-[[2,2'-bis(methoxymethoxy)-7,7'-bis(phenylmethoxy)[1,1'-
binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (R)- (9CI) (CA INDEX
NAME)



09/893,680

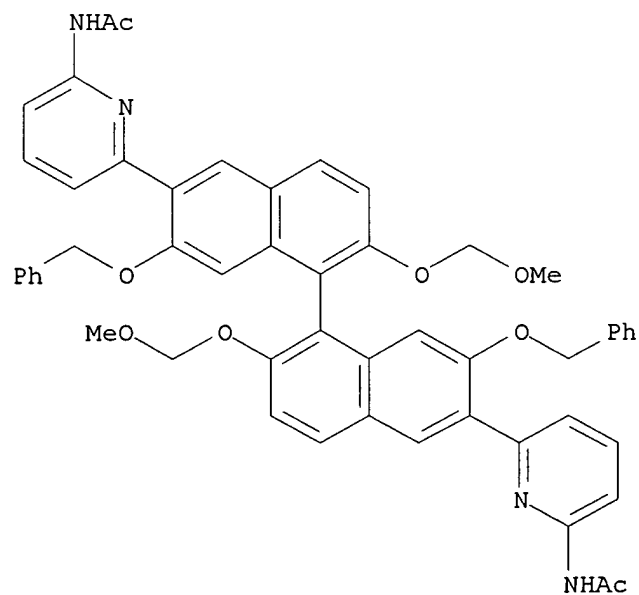
RN 205940-06-3 CAPLUS

CN Acetamide, N,N'-[[2,2'-dihydroxy-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (R)- (9CI) (CA INDEX NAME)



RN 205940-13-2 CAPLUS

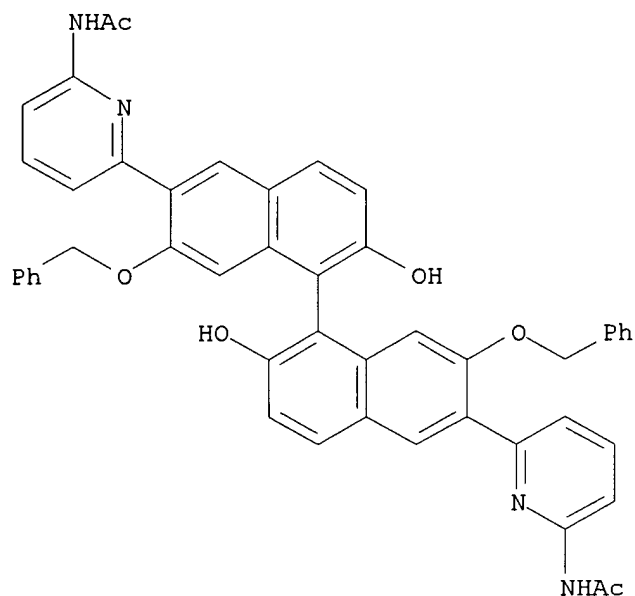
CN Acetamide, N,N'-[[2,2'-bis(methoxymethoxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (S)- (9CI) (CA INDEX NAME)



09/893,680

RN 205940-14-3 CAPLUS

CN Acetamide, N,N'-[[2,2'-dihydroxy-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (S)- (9CI) (CA INDEX NAME)

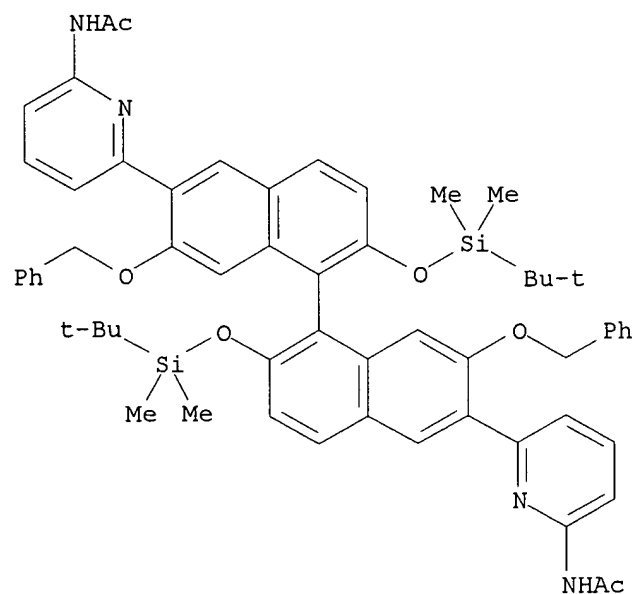


IT 205940-10-9P 205940-11-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and enantioselective excitatory amino acid recognition of
bis(pyridinediylacetamide)binaphthalene receptors)

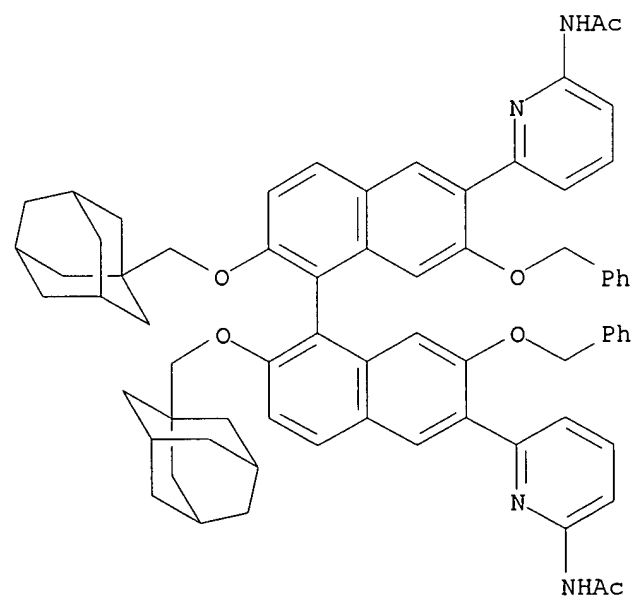
RN 205940-10-9 CAPLUS

CN Acetamide, N,N'-[[2,2'-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (S)- (9CI) (CA INDEX NAME)

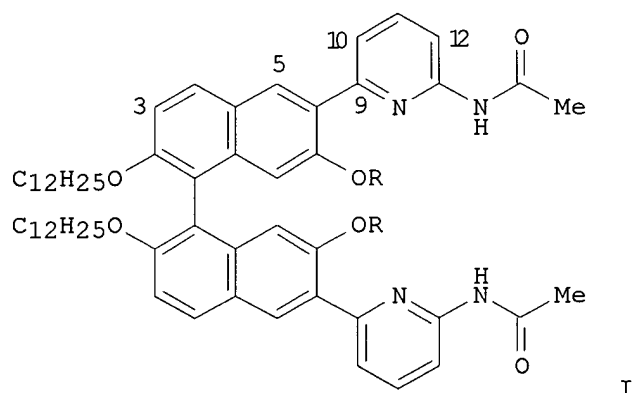


RN 205940-11-0 CAPLUS

CN Acetamide, N,N'-[[2,2'-bis(tricyclo[3.3.1.1^{3,7}]dec-1-ylmethoxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (S)- (9CI) (CA INDEX NAME)



L19 ANSWER 5 OF 21 CAPLUS COPYRIGHT 2002 ACS
 AN 1995:834662 CAPLUS
 DN 124:56600
 TI Chiral 1,1'-binaphthyl molecular clefts for the complexation of excitatory amino-acid derivatives
 AU Martinborough, Esther; Denti, Tiziana Modasini; Castro, Peter P.; Wyman, Tara B.; Knobler, Carolyn B.; Diederich, Francois
 CS Lab. Org. Chem., Eidgenoessichen Tech. Hochschule, Zurich, CH08092, Switz.
 SO Helvetica Chimica Acta (1995), 78(5), 1037-66
 CODEN: HCACAV; ISSN: 0018-019X
 PB Verlag Helvetica Chimica Acta
 DT Journal
 LA English
 OS CASREACT 124:56600
 GI



AB The complexation of N-Cbz derivs. of Asp, Glu, and L-kainic acid was studied in CDCl₃ with various chiral receptors consisting of a 1,1'-binaphthyl spacer with (carboxamido)pyridine functionality at the 6,6'-positions in the major groove. Receptors of type A possess 2 N-(pyridin-2-yl)carboxamide H-bonding sites, whereas type B-receptors have 2 N-(pyridine-2,6-diyl)acetamide residues attached. Complexes of excitatory amino-acid derivs. and other, achiral .alpha.,.omega.-dicarboxylic acids with these receptors are primarily stabilized by 2 sets of C:O.cntdot..cntdot..cntdot.H-N and O-H.cntdot..cntdot..cntdot.N H-bonds. Optically active type-A receptors showed a preference for the large Glu deriv., whereas type-B receptors formed more stable complexes with the smaller Cbz-Asp. To improve the poor enantioselectivity addnl. functionality was introduced at the 7,7'-positions of the 1,1'-binaphthyl spacer, and the nature of the H-bonding sites in the 6,6'-positions was varied. (.+-.)-I [R = CH₂Ph, Me] formed the most stable complexes with dicarboxylic acids, and these receptors were synthesized in enantiomerically pure form. By 1H NMR binding titrns., the complexation of (R)- and (S)-I with the excitatory amino-acid derivs. was studied in CDCl₃, and assocn. consts. of K_a = 10³ - 2 .times. 10⁵ L.cntdot.mmol⁻¹ were measured for the 1:1 host-guest complexes. Enantioselective binding was limited to I [R = CH₂Ph], with the (R)-enantiomer complexing Cbz-Asp

by 0.7 kcal.cntdot.mol⁻¹ more tightly than the (S)-enantiomer. An unusual variety of interesting arom. interactions and secondary electrostatic interactions are responsible for the high binding affinity and the enantioselection obsd. with (R)- and (S)-I [R = CH₂Ph]. To enhance the enantioselectivity by reducing the conformational flexibility of the 1,1'-binaphthyl spacer, an addnl. crown-ether binding site was attached to the 2,2'-positions in the minor groove of type-B receptors. The binding affinity and the enantioselectivity were not altered upon complexation of Hg(CN)₂ at the crown-ether binding site, demonstrating lack of cooperativity between the minor- and major-groove recognition sites.

IT 171976-53-7P 171976-54-8P 171976-59-3P
 171976-60-6P 171976-61-7P 171976-62-8P
 171976-63-9P 171976-64-0P 171976-65-1P
 171976-66-2P 171976-67-3P 171976-68-4P
 171976-69-5P 171976-70-8P 171976-71-9P
 171976-90-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (assocn. consts. and prepn. of chiral 1,1'-binaphthyl mol. clefts with
 .alpha.,.omega.-dicarboxylic acid recognition sites)

RN 171976-53-7 CAPLUS

RN 171976-54-8 CAPLUS

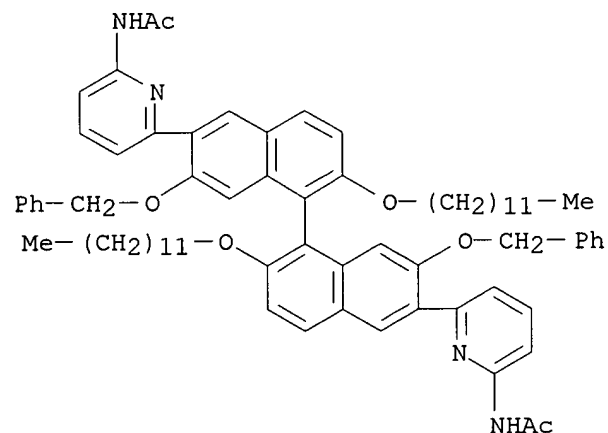
RN 171976-59-3 CAPLUS

CN Butanedioic acid, 2,2-diphenyl-, compd. with N,N'-[[2,2'-bis(dodecyloxy)-
 7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-
 pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171976-26-4

CMF C72 H86 N4 O6

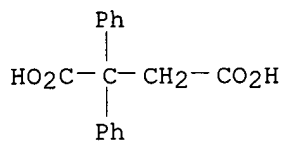


CM 2

CRN 10186-26-2

CMF C16 H14 O4

09/893,680



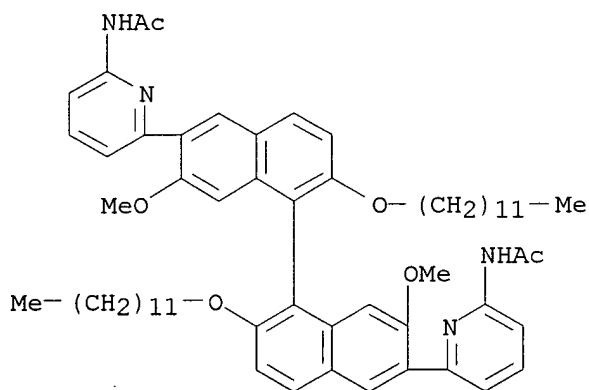
RN 171976-60-6 CAPLUS

CN Butanedioic acid, 2,2-diphenyl-, compd. with N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171976-29-7

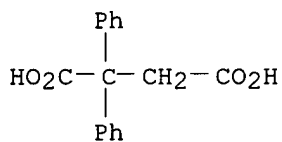
CMF C60 H78 N4 O6



CM 2

CRN 10186-26-2

CMF C16 H14 O4



RN 171976-61-7 CAPLUS

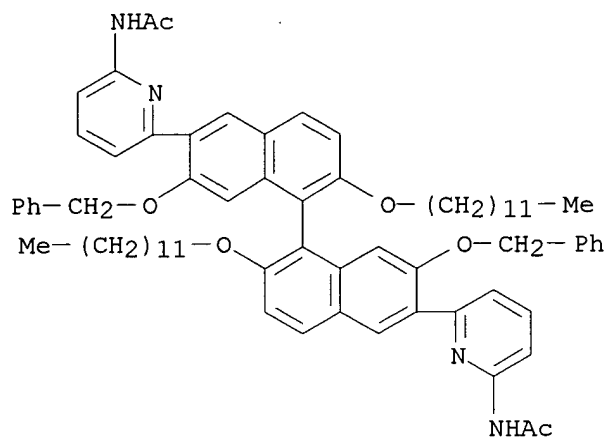
CN Pentanedioic acid, compd. with N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171976-26-4

CMF C72 H86 N4 O6

09/893,680



CM 2

CRN 110-94-1

CMF C5 H8 O4

HO₂C-(CH₂)₃-CO₂H

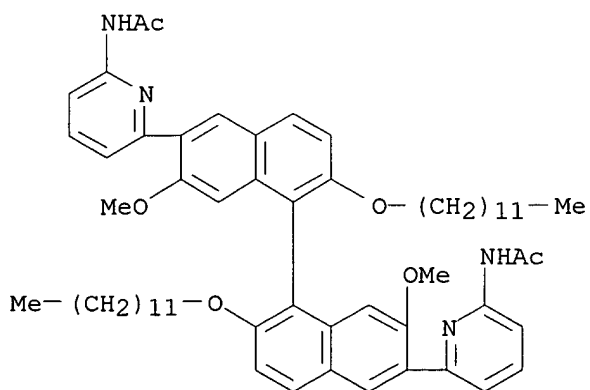
RN 171976-62-8 CAPLUS

CN Pentanedioic acid, compd. with N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171976-29-7

CMF C60 H78 N4 O6



CM 2

09/893,680

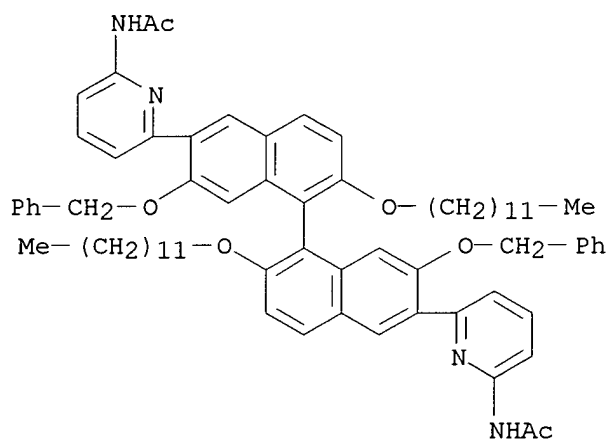
CRN 110-94-1
CMF C5 H8 O4

$\text{HO}_2\text{C}-(\text{CH}_2)_3-\text{CO}_2\text{H}$

RN 171976-63-9 CAPLUS
CN Pentanedioic acid, monomethyl ester, compd. with N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

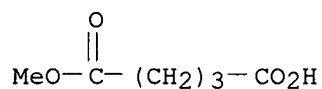
CM 1

CRN 171976-26-4
CMF C72 H86 N4 O6



CM 2

CRN 1501-27-5
CMF C6 H10 O4

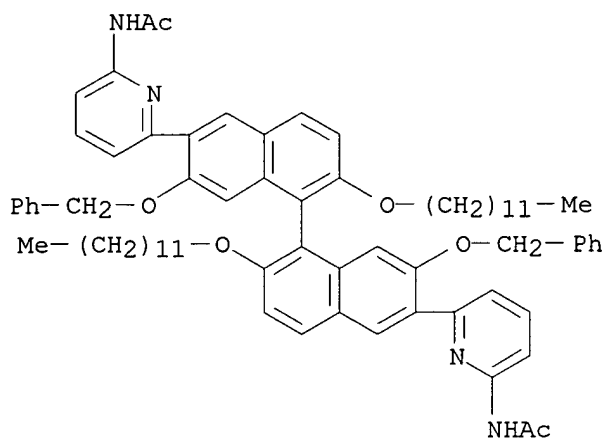


RN 171976-64-0 CAPLUS
CN Heptanedioic acid, compd. with N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171976-26-4
CMF C72 H86 N4 O6

09/893,680



CM 2

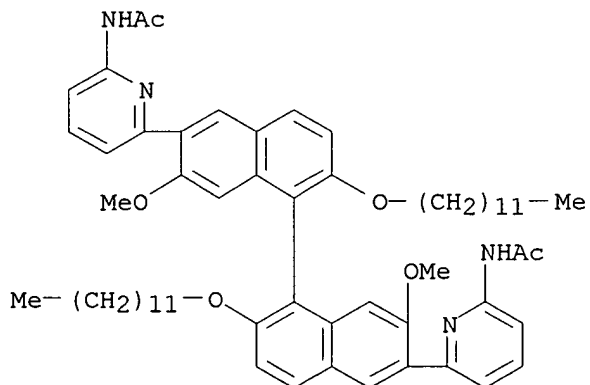
CRN 111-16-0
CMF C7 H12 O4

HO₂C-(CH₂)₅-CO₂H

RN 171976-65-1 CAPLUS
CN Heptanedioic acid, compd. with N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171976-29-7
CMF C60 H78 N4 O6



CM 2

09/893,680

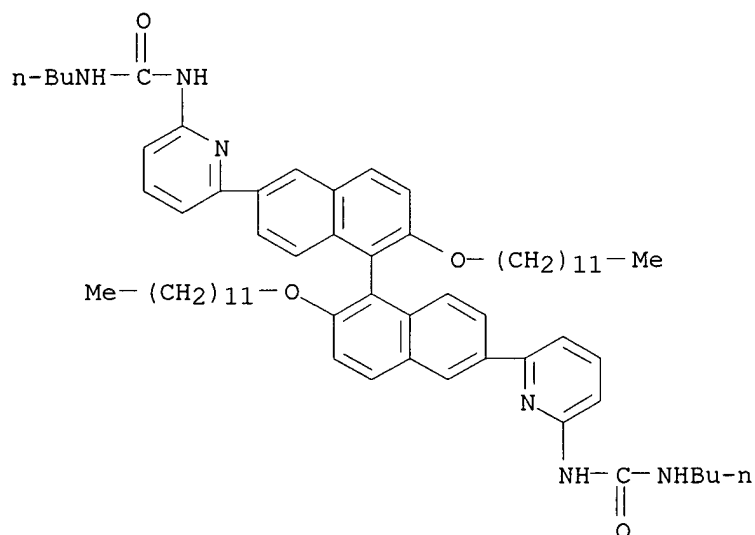
CRN 111-16-0
CMF C7 H12 O4

HO₂C-(CH₂)₅-CO₂H

RN 171976-66-2 CAPLUS
CN Heptanedioic acid, compd. with N,N'-[[2,2'-bis(dodecyloxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[N'-butylurea] (1:1) (9CI)
(CA INDEX NAME)

CM 1

CRN 171976-34-4
CMF C64 H88 N6 O4



CM 2

CRN 111-16-0
CMF C7 H12 O4

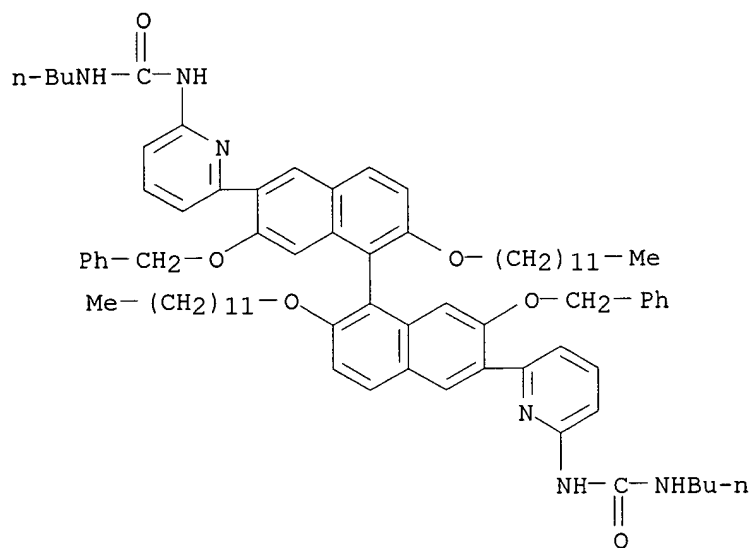
HO₂C-(CH₂)₅-CO₂H

RN 171976-67-3 CAPLUS
CN Heptanedioic acid, compd. with N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[N'-butylurea] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171976-35-5
CMF C78 H100 N6 O6

09/893,680



CM 2

CRN 111-16-0
CMF C7 H12 O4

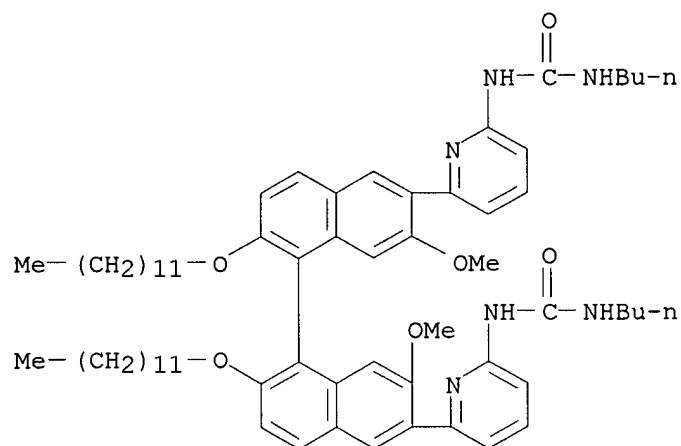
$\text{HO}_2\text{C}-(\text{CH}_2)_5-\text{CO}_2\text{H}$

RN 171976-68-4 CAPLUS
CN Heptanedioic acid, compd. with N,N''-[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-dinaphthaene]-6,6'-diyl]di-6,2-pyridinediyl]bis[N'-butylurea] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171976-36-6
CMF C66 H92 N6 O6

09/893,680



CM 2

CRN 111-16-0
CMF C7 H12 O4

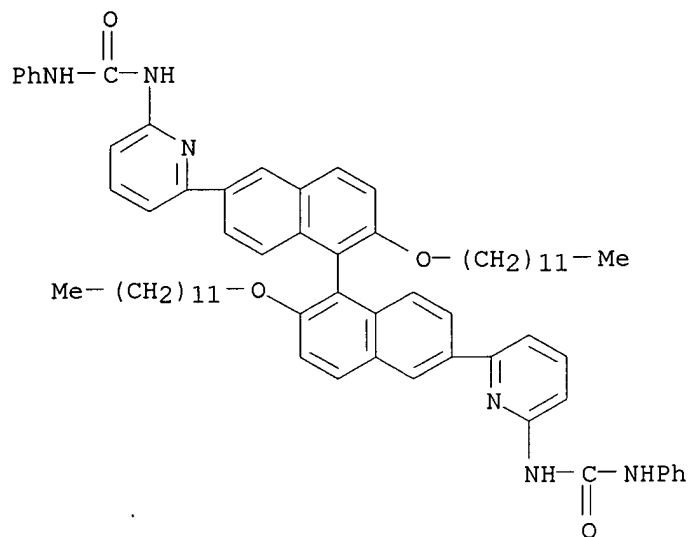
HO₂C-(CH₂)₅-CO₂H

RN 171976-69-5 CAPLUS
CN Heptanedioic acid, compd. with N,N'-[[2,2'-(dodecyloxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[N'-phenylurea] (1:1)
(9CI) (CA INDEX NAME)

CM 1

CRN 171976-38-8
CMF C68 H80 N6 O4

09/893,680



CM 2

CRN 111-16-0
CMF C7 H12 O4

HO₂C-(CH₂)₅-CO₂H

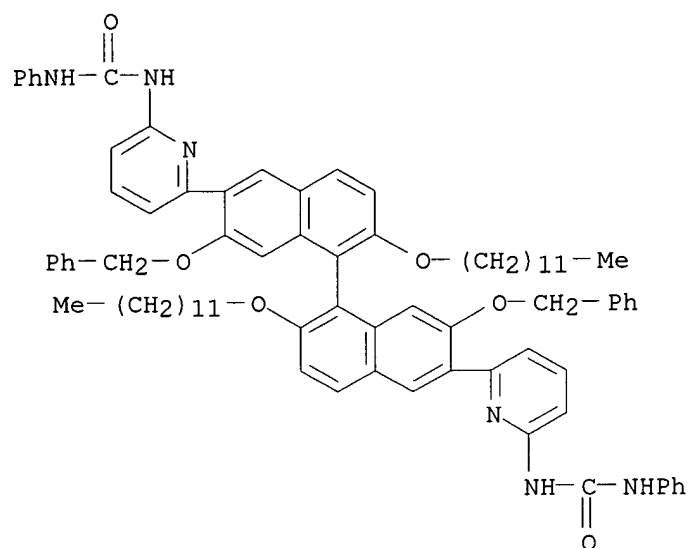
RN 171976-70-8 CAPLUS

CN Heptanedioic acid, compd. with N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[N'-phenylurea] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171976-39-9
CMF C82 H92 N6 O6

09/893,680



CM 2

CRN 111-16-0
CMF C7 H12 O4

HO₂C-(CH₂)₅-CO₂H

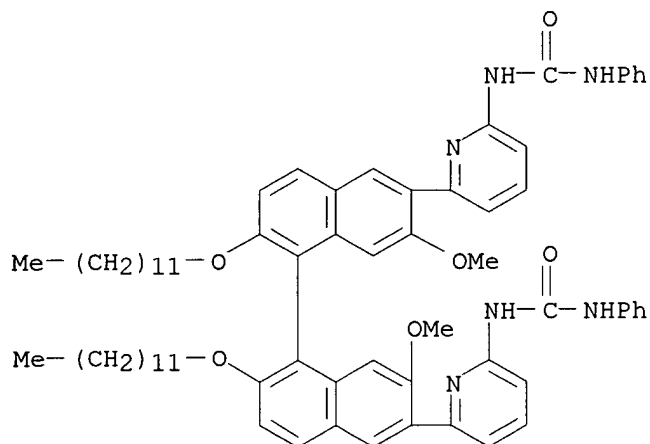
RN 171976-71-9 CAPLUS

CN Heptanedioic acid, compd. with N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[N'-phenylurea] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171976-40-2
CMF C70 H84 N6 O6

09/893,680



CM 2

CRN 111-16-0
CMF C7 H12 O4

HO₂C-(CH₂)₅-CO₂H

RN 171976-90-2 CAPLUS

IT 171976-47-9P 171976-48-0P 171976-49-1P
171976-50-4P 171976-73-1P 171976-74-2P
171976-75-3P 171976-76-4P 171976-77-5P
171976-78-6P 171976-79-7P 171976-80-0P
171976-81-1P 171976-82-2P 172139-13-8P
172139-14-9P 172139-15-0P 172139-16-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of chiral 1,1'-binaphthyl mol. clefts for complexation of
excitatory amino-acid derivs.)

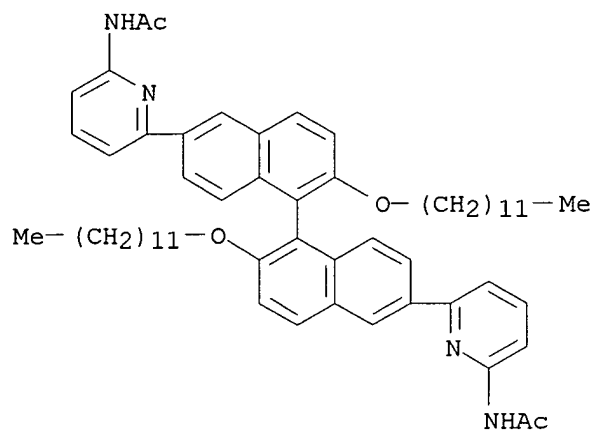
RN 171976-47-9 CAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(R)-N,N'-[[2,2'-bis(dodecyloxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-
pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 171976-21-9
CMF C58 H74 N4 O4
CDES 1:R

09/893,680



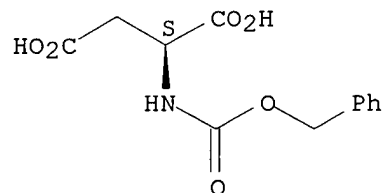
CM 2

CRN 1152-61-0

CMF C12 H13 N O6

CDES 5:L

Absolute stereochemistry.



RN 171976-48-0 CAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(S)-N,N'-[[2,2'-bis(dodecyloxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-
pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

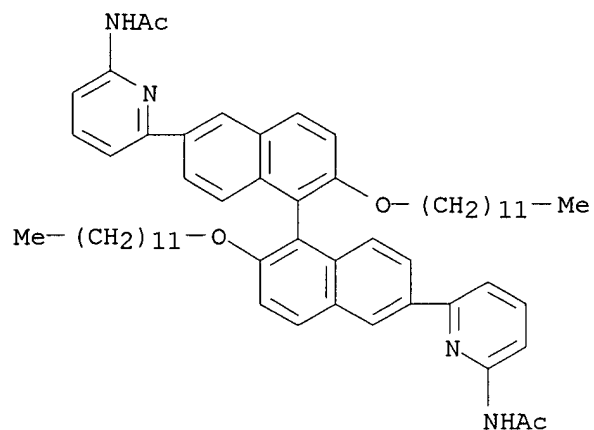
CM 1

CRN 171976-22-0

CMF C58 H74 N4 O4

CDES 1:S

09/893,680



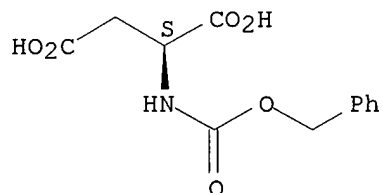
CM 2

CRN 1152-61-0

CMF C12 H13 N O6

CDES 5:L

Absolute stereochemistry.



RN 171976-49-1 CAPLUS

CN L-Glutamic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(R)-N,N'-[[2,2'-bis(dodecyloxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-
pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

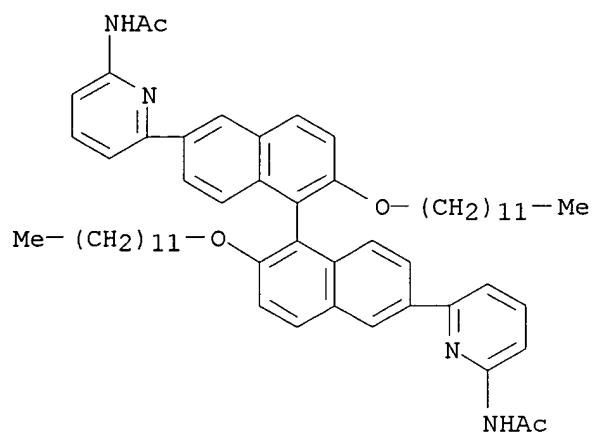
CM 1

CRN 171976-21-9

CMF C58 H74 N4 O4

CDES 1:R

09/893,680



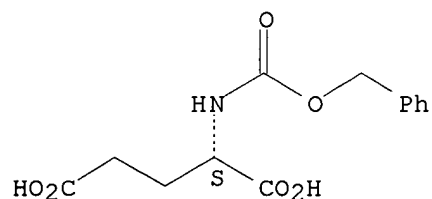
CM 2

CRN 1155-62-0

CMF C13 H15 N O6

CDES 5:L

Absolute stereochemistry.



RN 171976-50-4 CAPLUS

CN L-Glutamic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(S)-N,N'-[[2,2'-bis(dodecyloxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-
pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

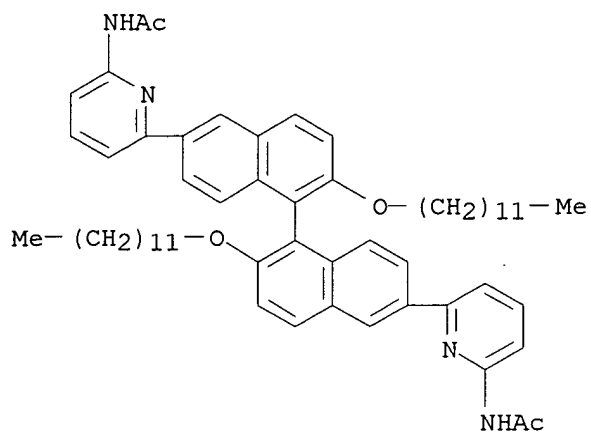
CM 1

CRN 171976-22-0

CMF C58 H74 N4 O4

CDES 1:S

09/893,680



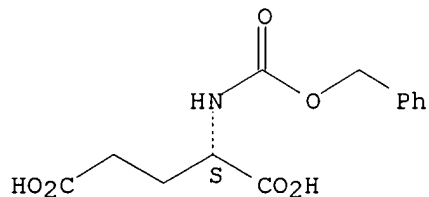
CM 2

CRN 1155-62-0

CMF C13 H15 N O6

CDES 5:L

Absolute stereochemistry.



RN 171976-73-1 CAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(R)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-
binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI)
(CA INDEX NAME)

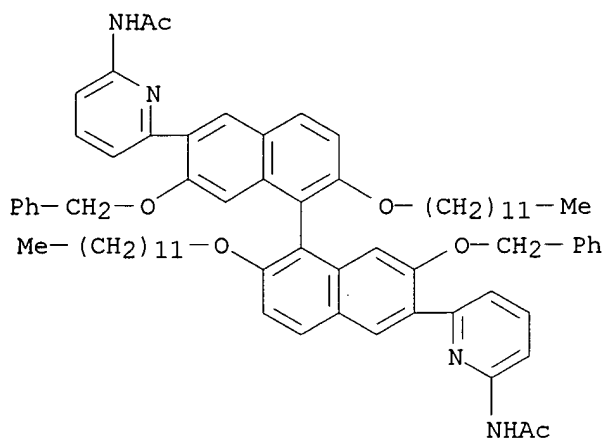
CM 1

CRN 171976-27-5

CMF C72 H86 N4 O6

CDES 1:R

09/893,680



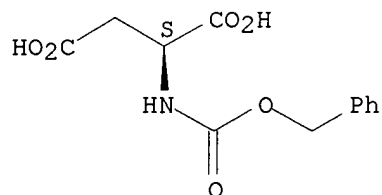
CM 2

CRN 1152-61-0

CMF C12 H13 N O6

CDES 5:L

Absolute stereochemistry.



RN 171976-74-2 CAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(S)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-
binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI)
(CA INDEX NAME)

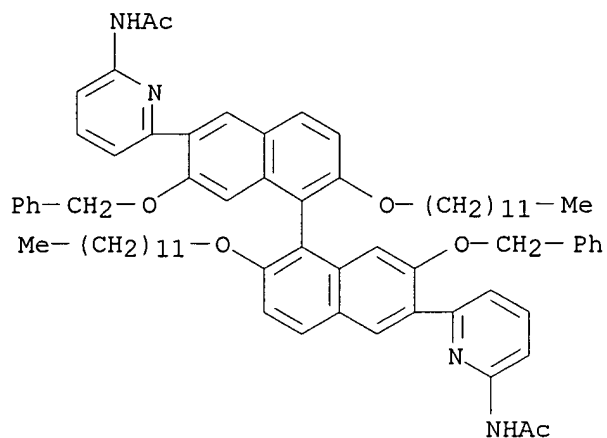
CM 1

CRN 171976-28-6

CMF C72 H86 N4 O6

CDES 1:S

09/893,680



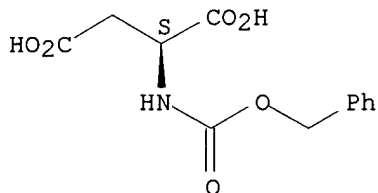
CM 2

CRN 1152-61-0

CMF C12 H13 N O6

CDES 5:L

Absolute stereochemistry.



RN 171976-75-3 CAPLUS

CN D-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(R)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-
binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI)
(CA INDEX NAME)

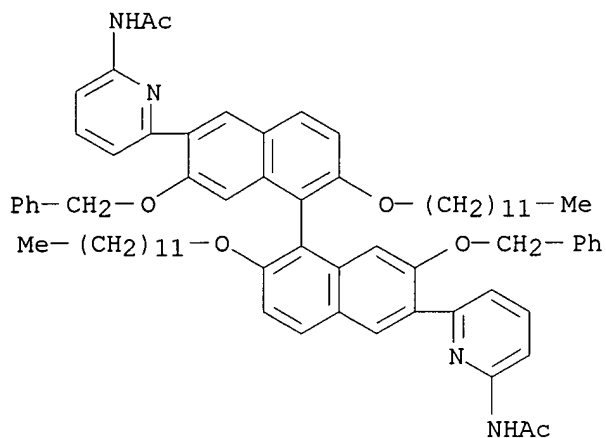
CM 1

CRN 171976-27-5

CMF C72 H86 N4 O6

CDES 1:R

09/893,680



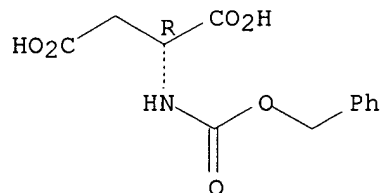
CM 2

CRN 78663-07-7

CMF C12 H13 N O6

CDES 5:D

Absolute stereochemistry.



RN 171976-76-4 CAPLUS

CN L-Glutamic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(R)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-
binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI)
(CA INDEX NAME)

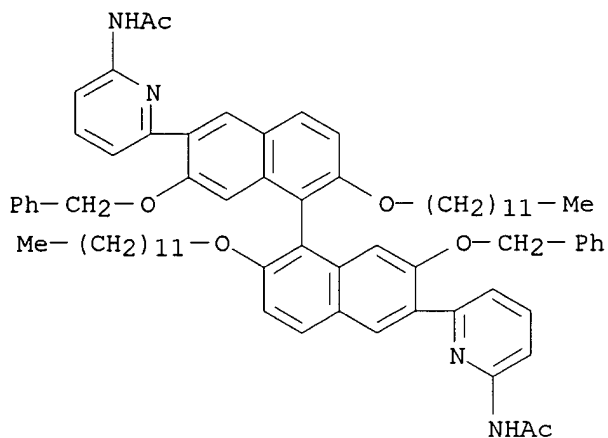
CM 1

CRN 171976-27-5

CMF C72 H86 N4 O6

CDES 1:R

09/893,680



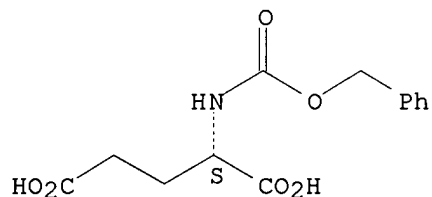
CM 2

CRN 1155-62-0

CMF C13 H15 N O6

CDES 5:L

Absolute stereochemistry.



RN 171976-77-5 CAPLUS

CN L-Glutamic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(S)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-
binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI)
(CA INDEX NAME)

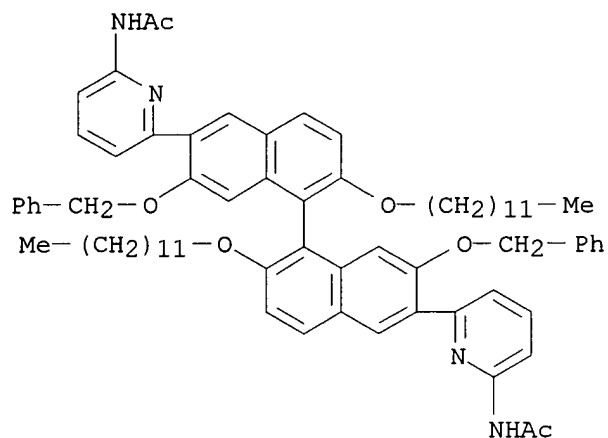
CM 1

CRN 171976-28-6

CMF C72 H86 N4 O6

CDES 1:S

09/893,680



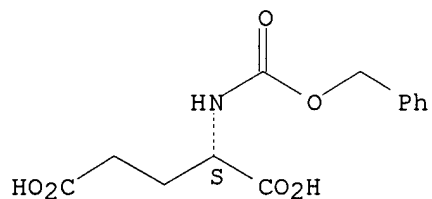
CM 2

CRN 1155-62-0

CMF C13 H15 N O6

CDES 5:L

Absolute stereochemistry.



RN 171976-78-6 CAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(R)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-
diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

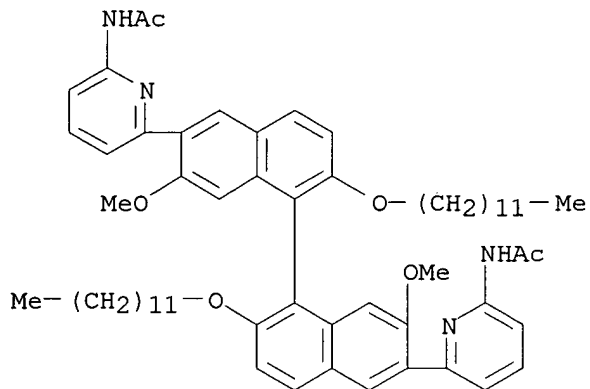
CM 1

CRN 171976-30-0

CMF C60 H78 N4 O6

CDES 1:R

09/893,680



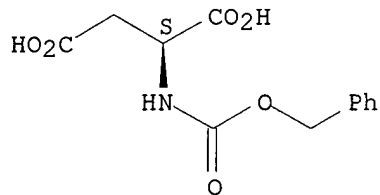
CM 2

CRN 1152-61-0

CMF C12 H13 N O6

CDES 5:L

Absolute stereochemistry.



RN 171976-79-7 CAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(S)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-
diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

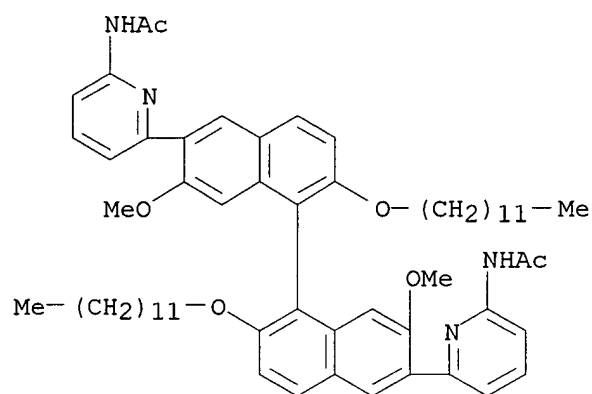
CM 1

CRN 171976-31-1

CMF C60 H78 N4 O6

CDES 1:S

09/893,680



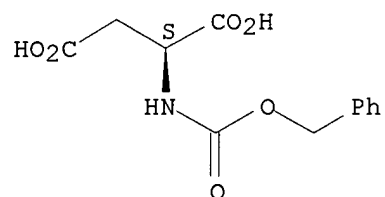
CM 2

CRN 1152-61-0

CMF C12 H13 N O6

CDES 5:L

Absolute stereochemistry.



RN 171976-80-0 CAPLUS

CN D-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(R)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-
diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

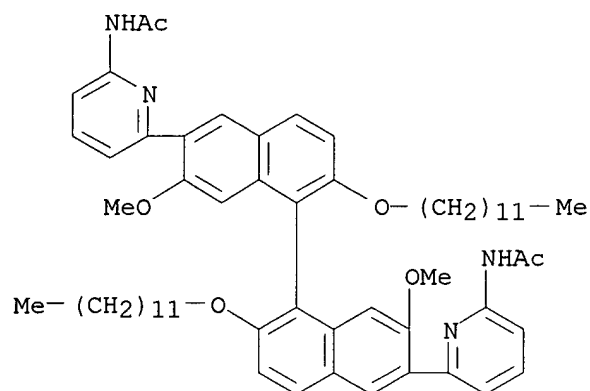
CM 1

CRN 171976-30-0

CMF C60 H78 N4 O6

CDES 1:R

09/893,680



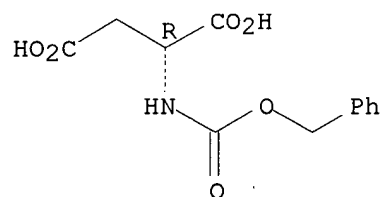
CM 2

CRN 78663-07-7

CMF C12 H13 N O6

CDES 5:D

Absolute stereochemistry.



RN 171976-81-1 CAPLUS

CN L-Glutamic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(R)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-
diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

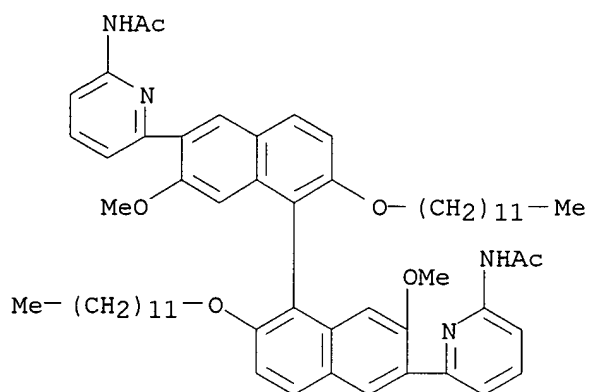
CM 1

CRN 171976-30-0

CMF C60 H78 N4 O6

CDES 1:R

09/893,680



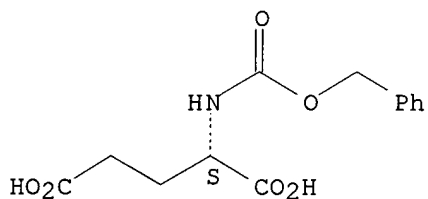
CM 2

CRN 1155-62-0

CMF C13 H15 N O6

CDES 5:L

Absolute stereochemistry.



RN 171976-82-2 CAPLUS

CN L-Glutamic acid, N-[(phenylmethoxy)carbonyl]-, compd. with
(S)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-
diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

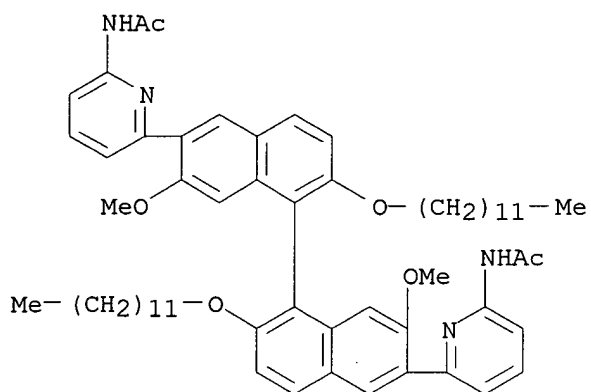
CM 1

CRN 171976-31-1

CMF C60 H78 N4 O6

CDES 1:S

09/893,680



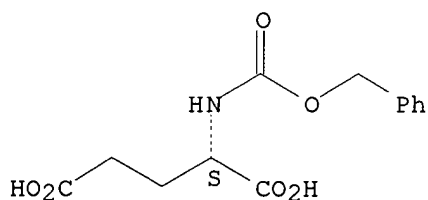
CM 2

CRN 1155-62-0

CMF C13 H15 N O6

CDES 5:L

Absolute stereochemistry.



RN 172139-13-8 CAPLUS

CN 1,2-Pyrrolidinedicarboxylic acid, 3-(carboxymethyl)-4-(1-methylethenyl)-, 1-(phenylmethyl) ester, [2S-(2.alpha.,3.beta.,4.beta.)]-, compd. with (R)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

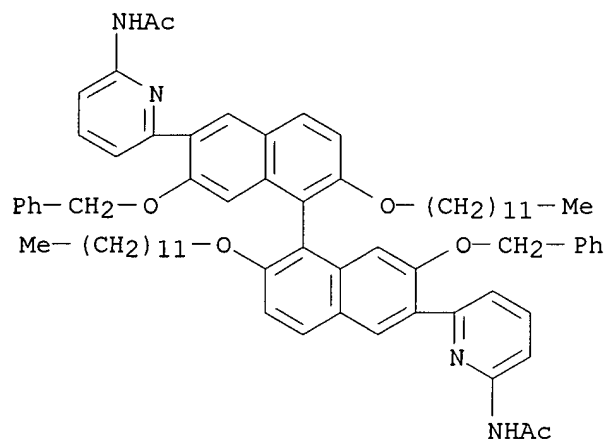
CM 1

CRN 171976-27-5

CMF C72 H86 N4 O6

CDES 1:R

09/893,680



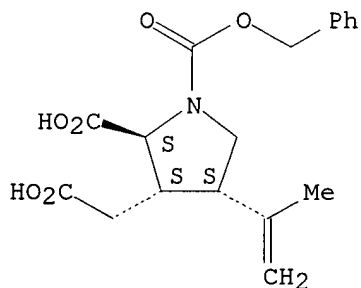
CM 2

CRN 73903-33-0

CMF C18 H21 N O6

CDES 1:2S2:2A,3B,4B

Absolute stereochemistry.



RN 172139-14-9 CAPLUS

CN 1,2-Pyrrolidinedicarboxylic acid, 3-(carboxymethyl)-4-(1-methylethenyl)-, 1-(phenylmethyl) ester, [2S-(2.alpha.,3.beta.,4.beta.)]-, compd. with (S)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

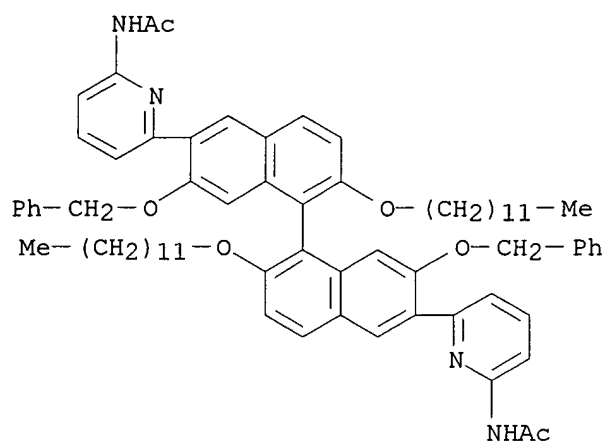
CM 1

CRN 171976-28-6

CMF C72 H86 N4 O6

CDES 1:S

09/893,680



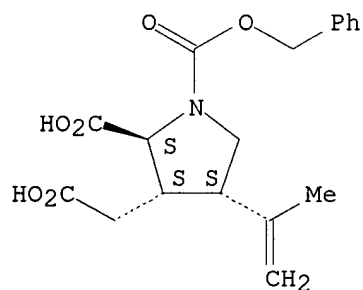
CM 2

CRN 73903-33-0

CMF C18 H21 N O6

CDES 1:2S2:2A,3B,4B

Absolute stereochemistry.



RN 172139-15-0 CAPLUS

CN 1,2-Pyrrolidinedicarboxylic acid, 3-(carboxymethyl)-4-(1-methylethenyl)-, 1-(phenylmethyl) ester, [2S-(2.alpha.,3.beta.,4.beta.)]-, compd. with (R)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

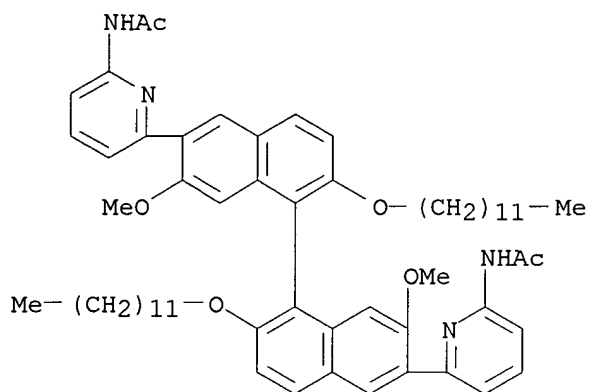
CM 1

CRN 171976-30-0

CMF C60 H78 N4 O6

CDES 1:R

09/893,680



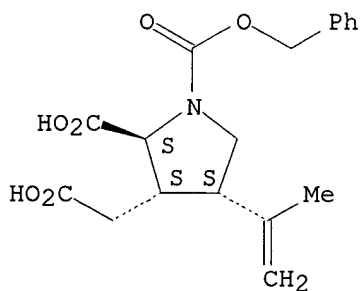
CM 2

CRN 73903-33-0

CMF C18 H21 N O6

CDES 1:2S2:2A,3B,4B

Absolute stereochemistry.



RN 172139-16-1 CAPLUS

CN 1,2-Pyrrolidinedicarboxylic acid, 3-(carboxymethyl)-4-(1-methylethenyl)-, 1-(phenylmethyl) ester, [2S-(2.alpha.,3.beta.,4.beta.)]-, compd. with (S)-N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

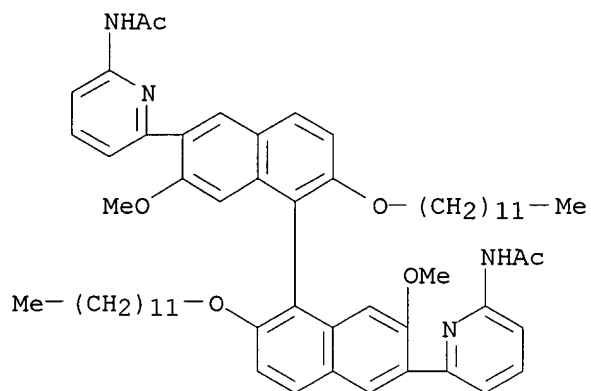
CM 1

CRN 171976-31-1

CMF C60 H78 N4 O6

CDES 1:S

09/893,680



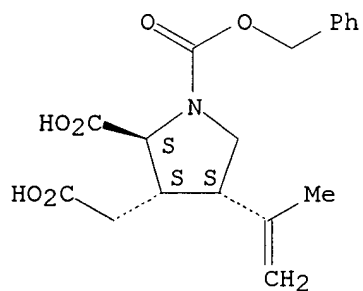
CM 2

CRN 73903-33-0

CMF C18 H21 N O6

CDES 1:2S2:2A,3B,4B

Absolute stereochemistry.



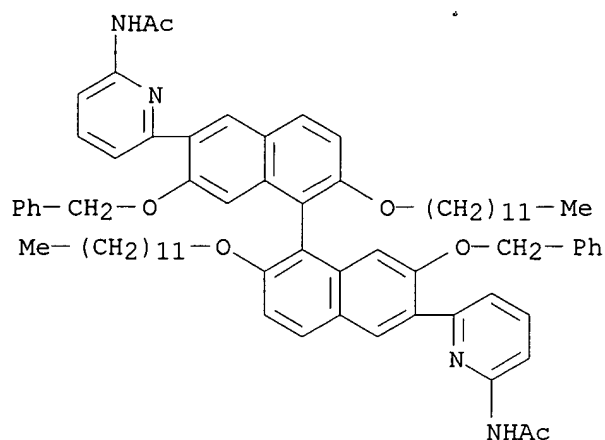
IT 171976-26-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of chiral 1,1'-binaphthyl mol. clefts for complexation of excitatory amino-acid derivs.)

RN 171976-26-4 CAPLUS

CN Acetamide, N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis- (9CI) (CA INDEX NAME)

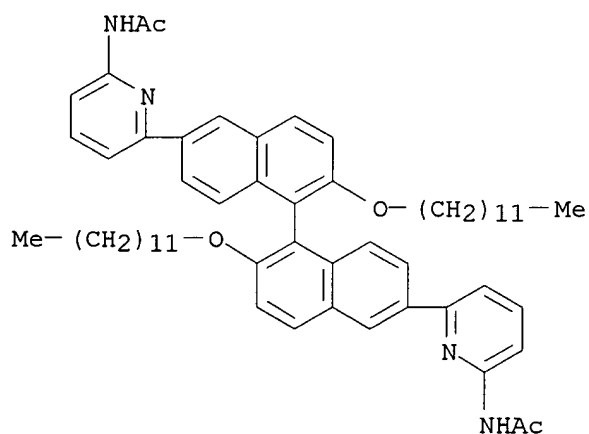


IT 171976-20-8P 171976-21-9P 171976-22-0P
 171976-27-5P 171976-28-6P 171976-29-7P
 171976-30-0P 171976-31-1P 171976-32-2P
 171976-34-4P 171976-35-5P 171976-36-6P
 171976-38-8P 171976-39-9P 171976-40-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of chiral 1,1'-binaphthyl mol. clefts for complexation of
 excitatory amino-acid derivs.)

RN 171976-20-8 CAPLUS

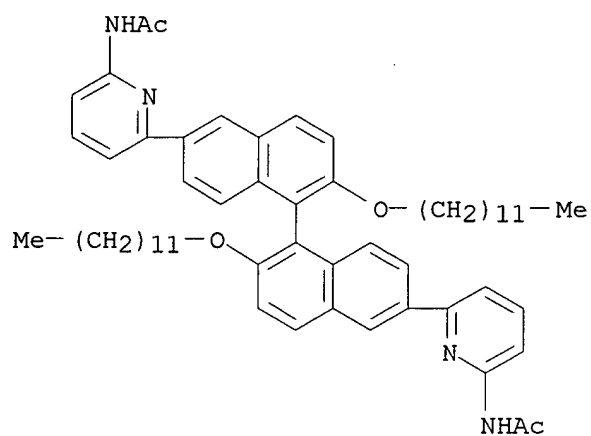
CN Acetamide, N,N'-[[2,2'-bis(dodecyloxy)[1,1'-binaphthalene]-6,6'-diyl]di-
 6,2-pyridinediyl]bis- (9CI) (CA INDEX NAME)



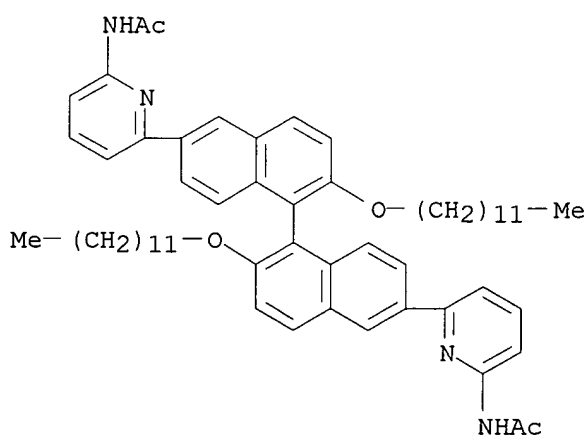
RN 171976-21-9 CAPLUS

CN Acetamide, N,N'-[[2,2'-bis(dodecyloxy)[1,1'-binaphthalene]-6,6'-diyl]di-
 6,2-pyridinediyl]bis-, (R)- (9CI) (CA INDEX NAME)

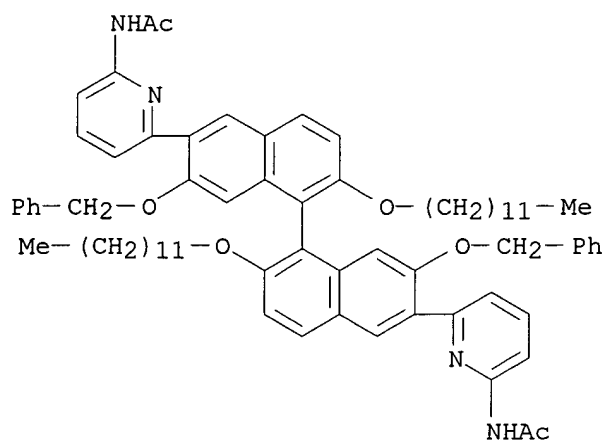
09/893,680



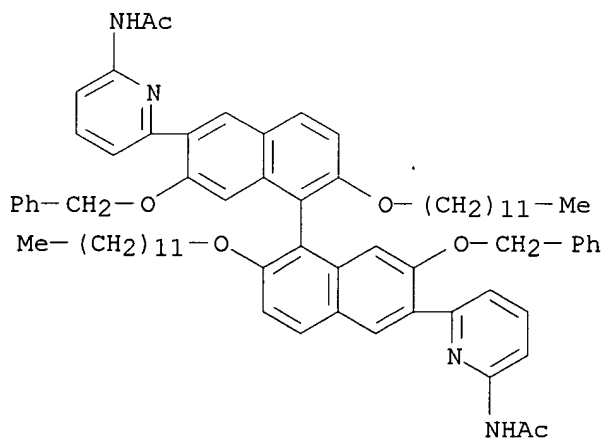
RN 171976-22-0 CAPLUS
CN Acetamide, N,N'-[[2,2'-bis(dodecyloxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (S)- (9CI) (CA INDEX NAME)



RN 171976-27-5 CAPLUS
CN Acetamide, N,N'-[[(1R)-2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis- (9CI) (CA INDEX NAME)

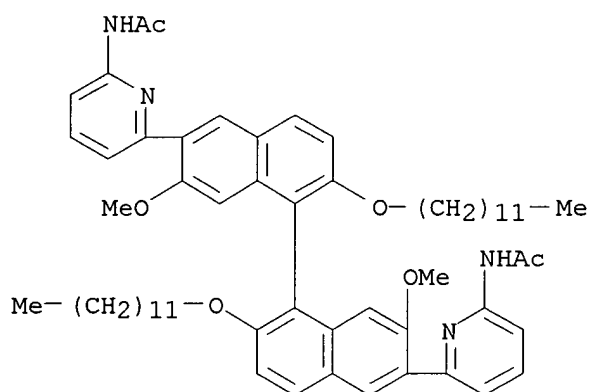


RN 171976-28-6 CAPLUS
 CN Acetamide, N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (S)- (9CI) (CA INDEX NAME)



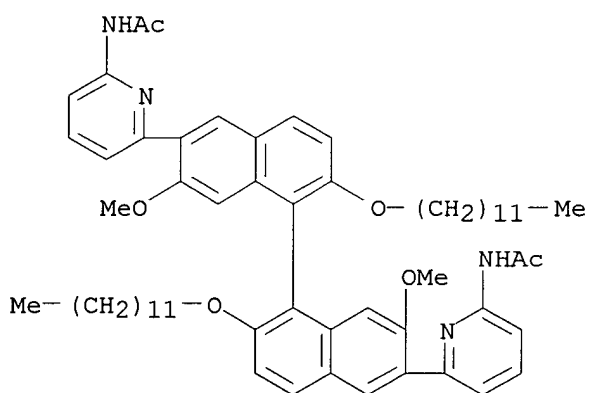
RN 171976-29-7 CAPLUS
 CN Acetamide, N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis- (9CI) (CA INDEX NAME)

09/893,680



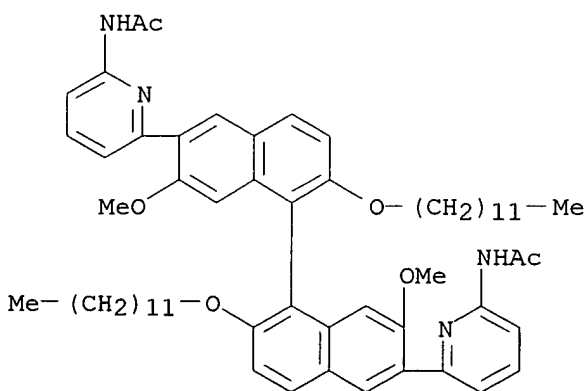
RN 171976-30-0 CAPLUS

CN Acetamide, N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (R)- (9CI) (CA INDEX NAME)



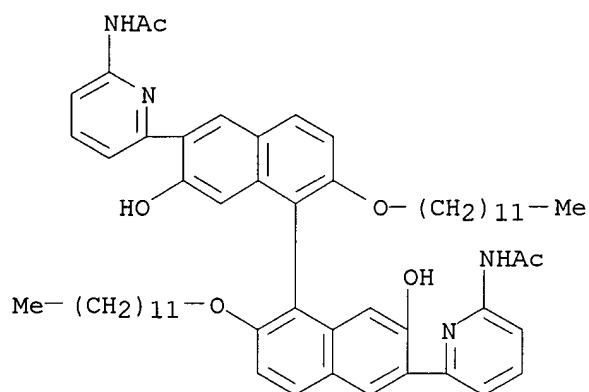
RN 171976-31-1 CAPLUS

CN Acetamide, N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis-, (S)- (9CI) (CA INDEX NAME)



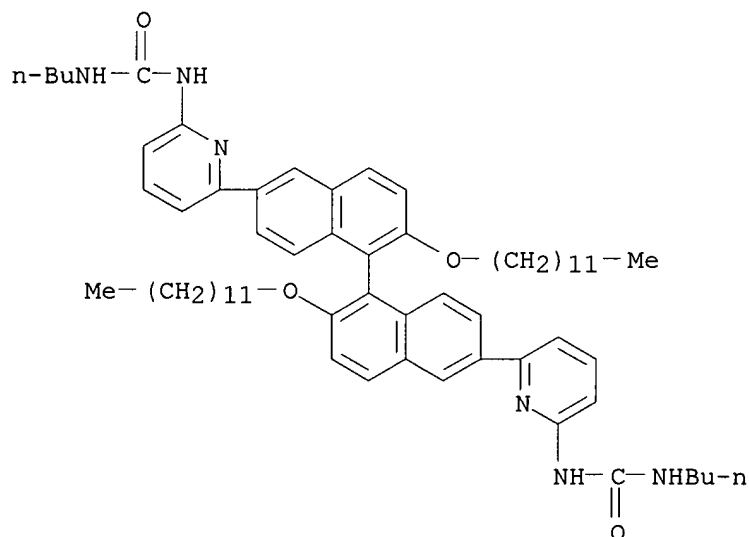
RN 171976-32-2 CAPLUS

CN Acetamide, N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dihydroxy[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis- (9CI) (CA INDEX NAME)



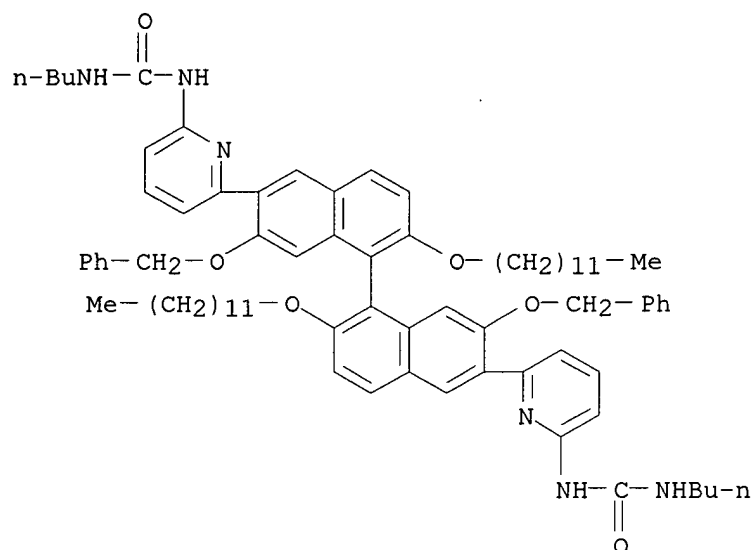
RN 171976-34-4 CAPLUS

CN Urea, N,N'-[[2,2'-bis(dodecyloxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[N'-butyl- (9CI) (CA INDEX NAME)



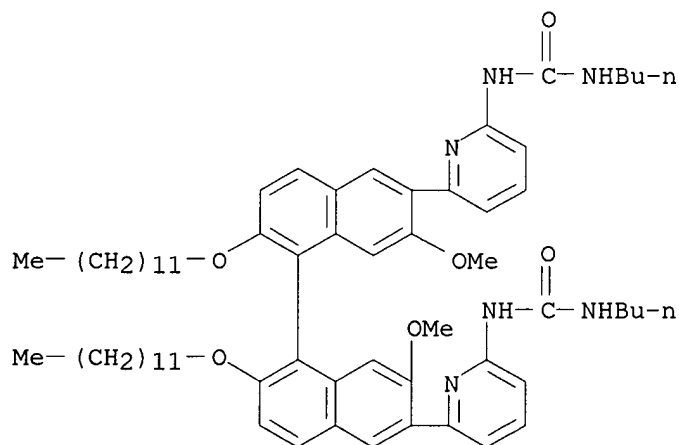
RN 171976-35-5 CAPLUS

CN Urea, N,N'-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[N'-butyl- (9CI) (CA INDEX NAME)



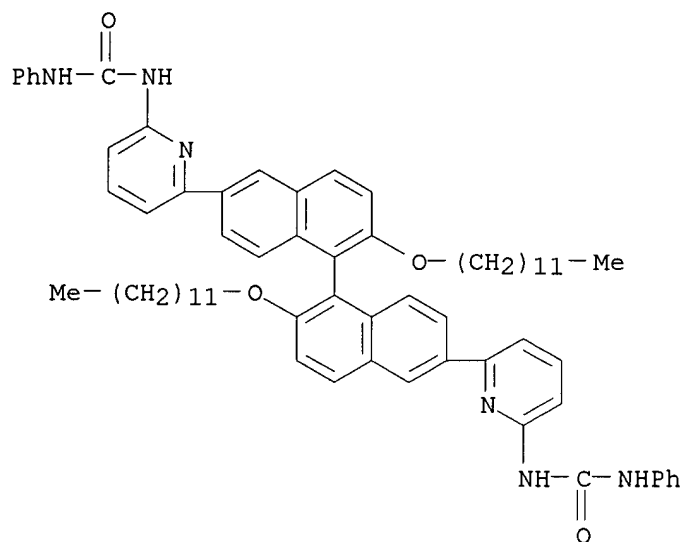
RN 171976-36-6 CAPLUS

CN Urea, N,N'-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[N'-butyl- (9CI) (CA INDEX NAME)

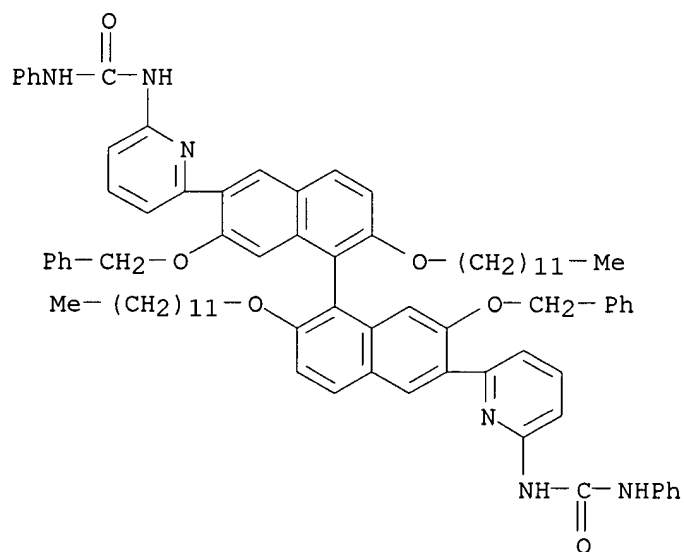


RN 171976-38-8 CAPLUS

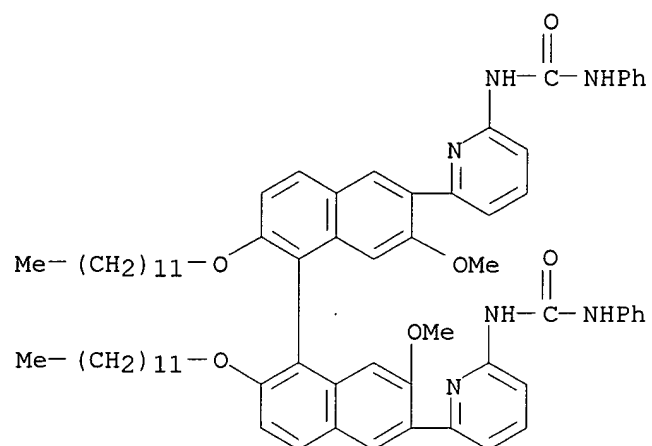
CN Urea, N,N'-[[2,2'-bis(dodecyloxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[N'-phenyl- (9CI) (CA INDEX NAME)



RN 171976-39-9 CAPLUS
 CN Urea, N,N''-[[2,2'-bis(dodecyloxy)-7,7'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[N'-phenyl- (9CI) (CA INDEX NAME)

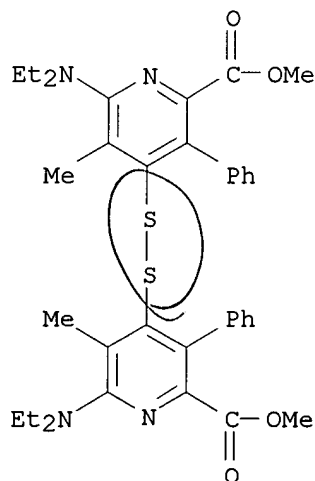


RN 171976-40-2 CAPLUS
 CN Urea, N,N''-[[2,2'-bis(dodecyloxy)-7,7'-dimethoxy[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[N'-phenyl- (9CI) (CA INDEX NAME)



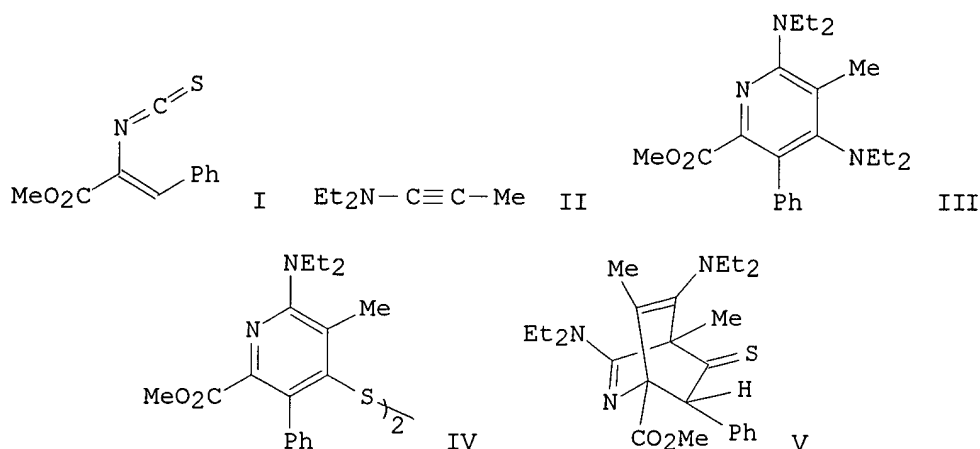
09/893,680

✓
19 ANSWER 6 OF 21 CAPLUS COPYRIGHT 2002 ACS
AN 1995:203025 CAPLUS
DN 122:81082
TI Synthesis of pentasubstituted pyridines. II. NMR study of the addition products of 1-(N,N-diethylamino)prop-1-yne to methyl 2-isothiocyanato-3-phenylpropenoate
AU Pelaez-Arango, Elvira; Lopez-Oritz, Fernando; Barluenga, Jose; Ferrero, Miguel; Palacios, Francisco
CS Instituto Univ. Quimica Organometalica Enrique Moles, Oviedo, 33071, Spain
SO Magnetic Resonance in Chemistry (1994), 32(11), 646-51
CODEN: MRCHEG; ISSN: 0749-1581
PB Wiley
DT Journal
LA English
AB The structure of the pentasubstituted pyridines obtained in the reaction of Me 2-isothiocyanato-3-phenylpropenoate with 1-(N,N-diethylamino)prop-1-yne were assigned based on 2D heteronuclear correlation expts. and NOE measurements. At 0.degree.C a 2-azabicyclo[2.2.2]octa-2,7-diene intermediate was isolated and spectroscopically characterized.
IT **156727-20-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 156727-20-7 CAPLUS
CN 2-Pyridinecarboxylic acid, 4,4'-dithiobis[6-(diethylamino)-5-methyl-3-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)



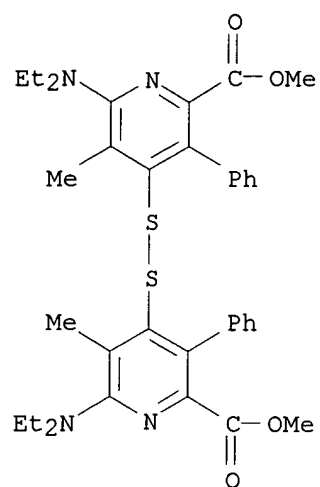
09/893,680

~~LI~~9 ANSWER 7 OF 21 CAPLUS COPYRIGHT 2002 ACS
AN 1994:508460 CAPLUS
DN 121:108460
TI A new domino synthesis of polyfunctionalized pentasubstituted pyridines
AU Barluenga, Jose; Ferrero, Miguel; Pelaez-Arango, Elvira; Lopez-Ortiz,
Fernando; Palacios, Francisco
CS Dep. Quim. Org., Univ. Oviedo, Oviedo, 33071, Spain
SO Journal of the Chemical Society, Chemical Communications (1994), (7),
865-6
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
OS CASREACT 121:108460
GI



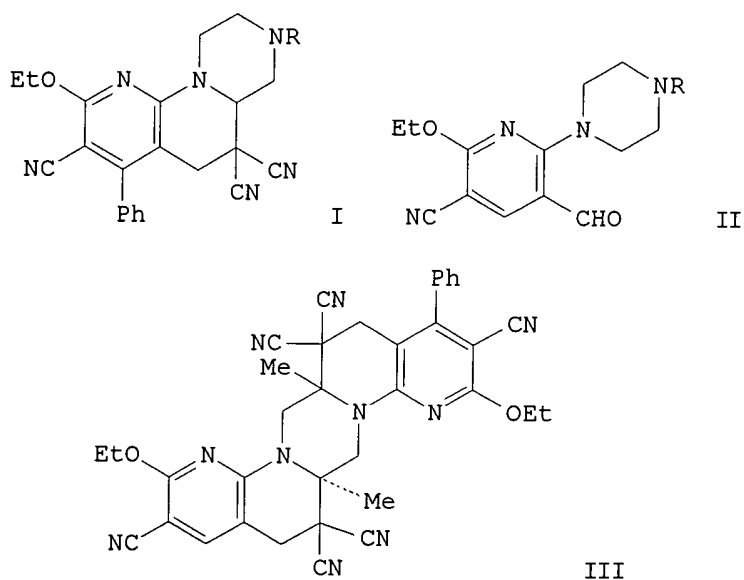
AB The reaction of N-vinylisocyanate (I) and ynamine (II) at 0-25 .degree.
affords pyridines III and IV regioselectivity; the intermediate
azanorbornadiene V has been isolated and spectroscopically characterized.
IT **156727-20-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 156727-20-7 CAPLUS
CN 2-Pyridinecarboxylic acid, 4,4'-dithiobis[6-(diethylamino)-5-methyl-3-
phenyl-, dimethyl ester (9CI) (CA INDEX NAME)

09/893,680



09/893,680

LI9 ANSWER 8 OF 21 CAPLUS COPYRIGHT 2002 ACS
AN 1993:671107 CAPLUS
DN 119:271107
TI Synthesis of pyrazino[1,2-a:4,5-a']di[1,8]naphthyridine and
pyrazino[1,2-a][1,8]naphthyridines
AU Ojea, Vicente; Quintela, Jose Maria
CS Fac. Cienc., Univ. La Coruna, La Coruna, 15071, Spain
SO Heterocycles (1993), 36(6), 1337-49
CODEN: HTCYAM; ISSN: 0385-5414
DT Journal
LA English
OS CASREACT 119:271107
GI



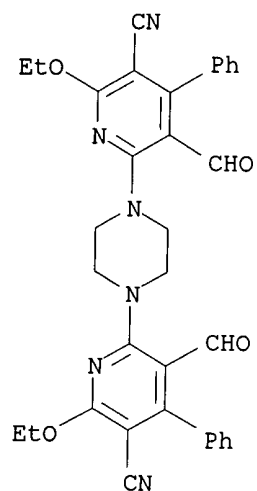
AB A series of 3-alkyl-, 3-aryl- and 3-hetarylhexasahydro-1H-pyrazino[1,2-a][1,8]naphthyridines [I; R = Me, CH₂Ph, CH₂CH₂C₆H₄CF₃-4, (un)substituted Ph, 2-pyridyl, etc.] were prepd. from 2-(4-substituted 1-piperazinyl)-3-formylpyridines (II) by condensation with malononitrile and subsequent thermal cyclization. Octahydro[1,2-a:4,5-a']di[1,8]naphthyridine (III) was also obtained.

IT **151021-40-8P 151021-41-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation of, with malononitrile)

RN 151021-40-8 CAPLUS

CN 3-Pyridinecarbonitrile, 6,6'-(1,4-piperazinediyl)bis[2-ethoxy-5-formyl-4-phenyl- (9CI) (CA INDEX NAME)

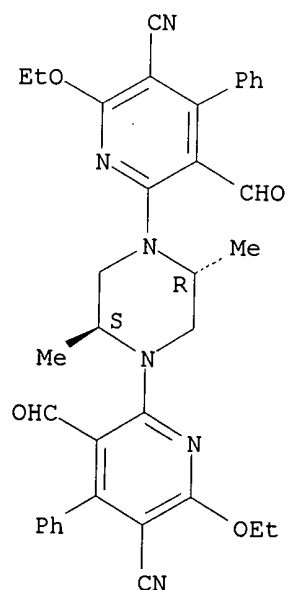
09/893,680



RN 151021-41-9 CAPLUS

CN 3-Pyridinecarbonitrile, 6,6'-(2,5-dimethyl-1,4-piperazinediyl)bis[2-ethoxy-5-formyl-4-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



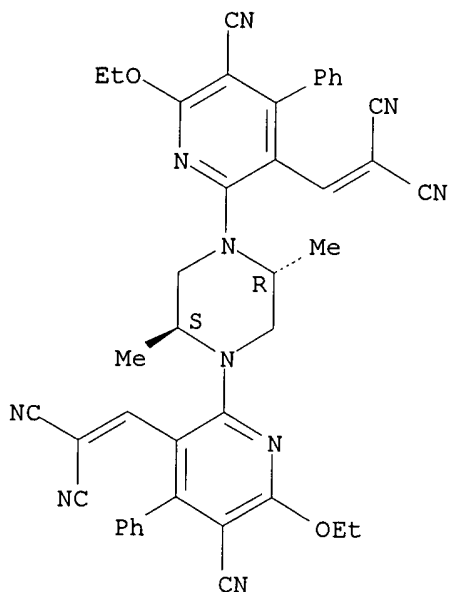
IT 151021-43-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of)

RN 151021-43-1 CAPLUS

CN Propanedinitrile, 2,2'-[(2,5-dimethyl-1,4-piperazinediyl)bis[(5-cyano-6-ethoxy-4-phenyl-2,3-pyridinediyl)methylidyne]]bis-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

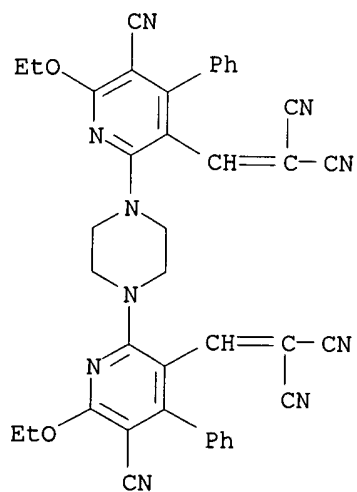


IT **151021-42-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 151021-42-0 CAPLUS

CN Propanedinitrile, 2,2'-[1,4-piperazinediylbis[(5-cyano-6-ethoxy-4-phenyl-2,3-pyridinediyl)methylidyne]]bis- (9CI) (CA INDEX NAME)



09/893,680

L18 ANSWER 9 OF 21 CAPLUS COPYRIGHT 2002 ACS
AN 1993:233206 CAPLUS
DN 118:233206
TI Chiral molecular clefts for dicarboxylic acid complexation
AU Alcazar, Victoria; Moran, Joaquin R.; Diederich, Francois
CS Dep. Chem. Biochem., Univ. California, Los Angeles, CA, 90024-1569, USA
SO Isr. J. Chem. (1992), 32(1), 69-77
CODEN: ISJCAT; ISSN: 0021-2148
DT Journal
LA English
OS CASREACT 118:233206
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Three efficient cleft-type receptors, I-III are prepd. by attachment of 2 amidopyridine units as H-bonding centers to either the 2,2'-positions of 9,9'-spirobifluorene or the 6,6'-positions of 1,1'-binaphthyl spacers. The easy availability of these compds. in short synthetic routes make them attractive complexing agents for aliph. and arom. dicarboxylic acids which undergo bidentate binding in CHCl₃. ¹H NMR binding studies show that substrates of different size can be accommodated into the clefts and form 1:1 complexes that are predominantly stabilized by multiple host-guest H-bonds. The flexible aliph. substrates diethylmalonic, 2,2-diphenylsuccinic, glutaric, and pimelic acid form complexes with assocn. consts. K_a ranging from 10³ to 10⁴ L mol⁻¹. Significantly more stable complexes (K_a > 10⁵ L mol⁻¹) are obtained with the more rigid, preorganized substrate 5-dodecyloxyisophthalic acid.

IT 147580-11-8 147580-12-9 147580-13-0

147580-14-1 147580-15-2

RL: PRP (Properties)
(formation const. of)

RN 147580-11-8 CAPLUS

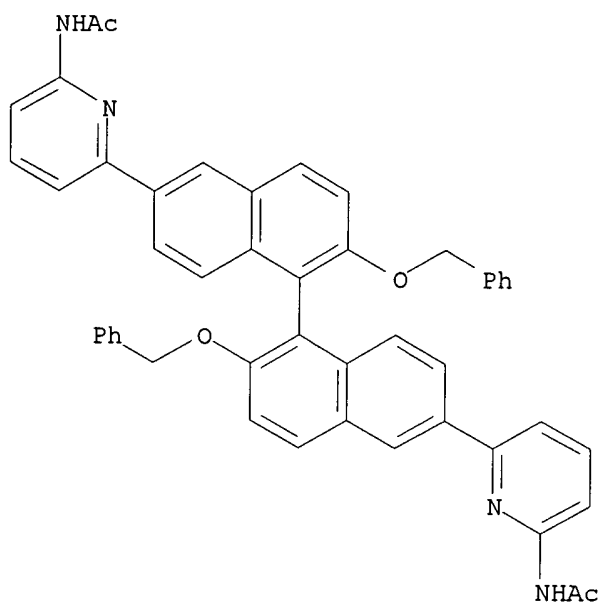
CN Propanedioic acid, diethyl-, compd. with N,N'-[[2,2'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147580-10-7

CMF C48 H38 N4 O4

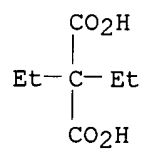
09/893,680



CM 2

CRN 510-20-3

CMF C7 H12 O4



RN 147580-12-9 CAPLUS

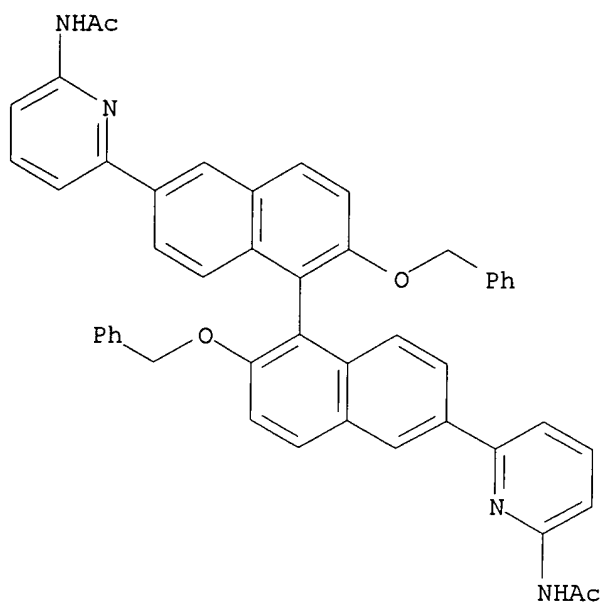
CN Butanedioic acid, 2,2-diphenyl-, compd. with N,N'-[[2,2'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147580-10-7

CMF C48 H38 N4 O4

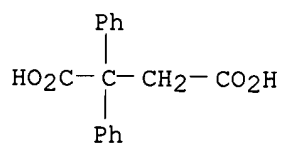
09/893,680



CM 2

CRN 10186-26-2

CMF C16 H14 O4



RN 147580-13-0 CAPLUS

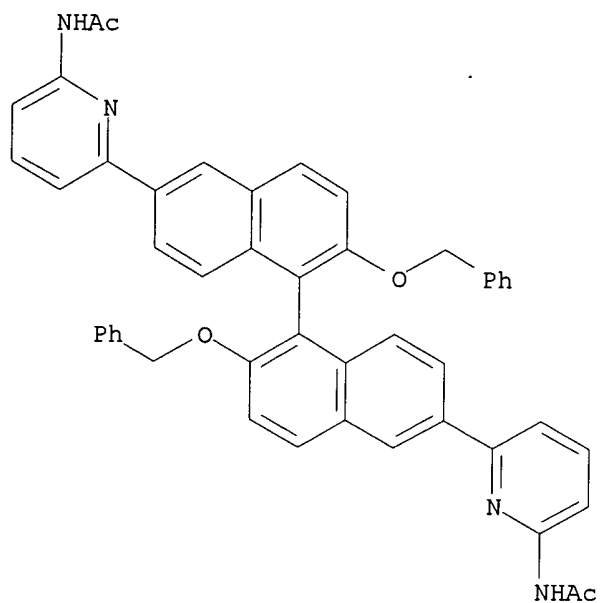
CN Pentanedioic acid, compd. with N,N'-[[2,2'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI)
(CA INDEX NAME)

CM 1

CRN 147580-10-7

CMF C48 H38 N4 O4

09/893,680



CM 2

CRN 110-94-1

CMF C5 H8 O4

HO₂C-(CH₂)₃-CO₂H

RN 147580-14-1 CAPLUS

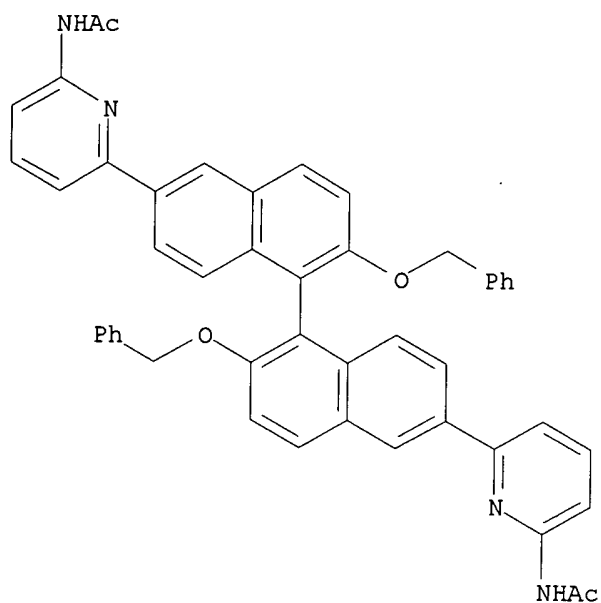
CN Heptanedioic acid, compd. with N,N'-[[2,2'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis[acetamide] (1:1) (9CI)
(CA INDEX NAME)

CM 1

CRN 147580-10-7

CMF C48 H38 N4 O4

09/893,680



CM 2

CRN 111-16-0

CMF C7 H12 O4

HO₂C-(CH₂)₅-CO₂H

RN 147580-15-2 CAPLUS

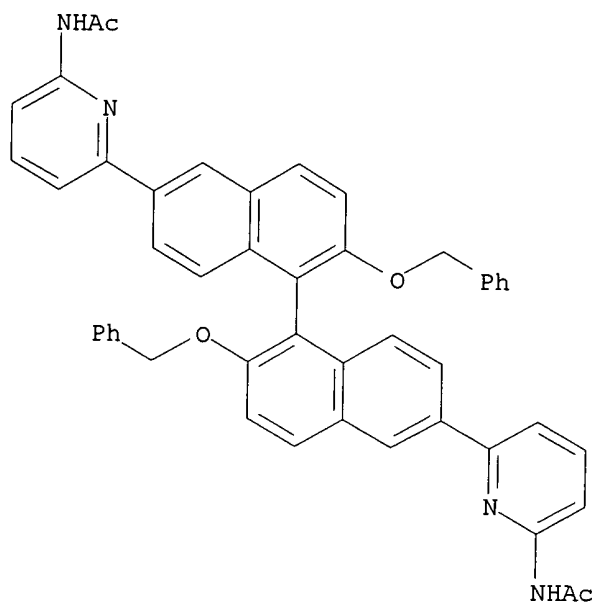
CN 1,3-Benzenedicarboxylic acid, 5-(dodecyloxy)-, compd. with
N,N'-[[2,2'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-
pyridinediyl]bis[acetamide] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147580-10-7

CMF C48 H38 N4 O4

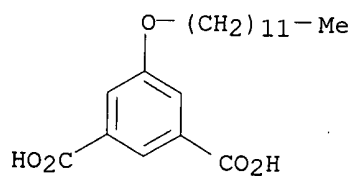
09/893,680



CM 2

CRN 147580-08-3

CMF C20 H30 O5



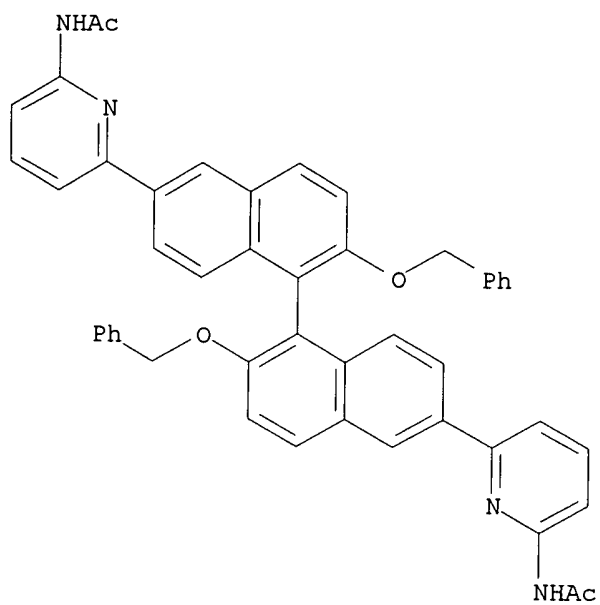
IT **147580-10-7**

RL: PRP (Properties)

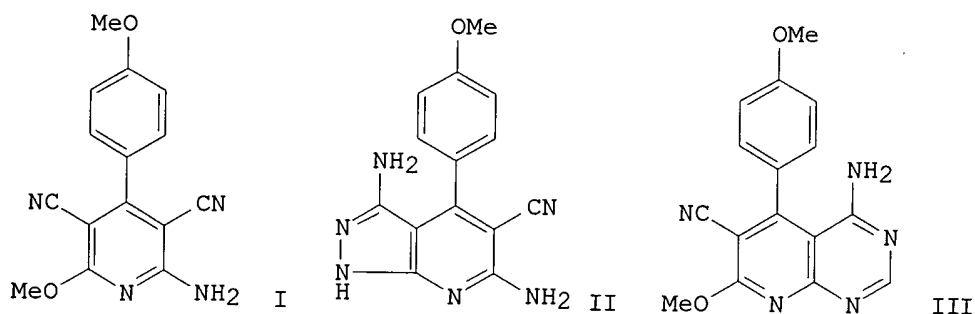
(prepn. as racemic mol. cleft receptor and proton NMR of)

RN 147580-10-7 CAPLUS

CN Acetamide, N,N'-[[2,2'-bis(phenylmethoxy)[1,1'-binaphthalene]-6,6'-diyl]di-6,2-pyridinediyl]bis- (9CI) (CA INDEX NAME)



~~L10~~ ANSWER 10 OF 21 CAPLUS COPYRIGHT 2002 ACS
~~AN~~ 1991:81740 CAPLUS
 DN 114:81740
 TI Reactions with 2-amino-3,5-dicyanopyridines
 AU Seada, M.; El-Behairy, M. A.; Jahine, H.; Hanafy, F.
 CS Fac. Educ., Ain Shams Univ., Cairo, Egypt
 SO Orient. J. Chem. (1989), 5(4), 273-80
 CODEN: OJCHEG; ISSN: 0970-020X
 DT Journal
 LA English
 OS CASREACT 114:81740
 GI



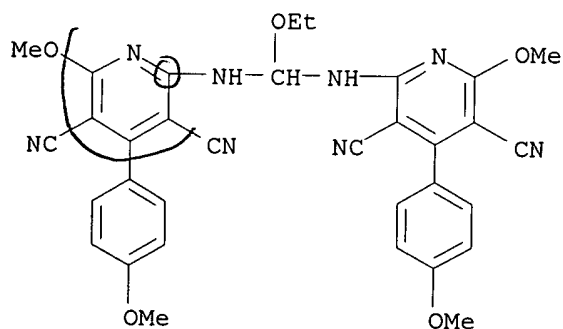
AB The prepn. and reactions of aminoanisylidicyanomethoxypyridine I and its
 derivs., e.g., pyrazolopyridine II, are described. Thus, $\text{CH}_2(\text{CN})_2$ reacted
 with 4-MeOC₆H₄CHO in the presence of MeONa in MeOH to give 60% I. I was
 boiled with HCONH₂ to give 91% pyridopyrimidine III.

IT **131695-27-7P**

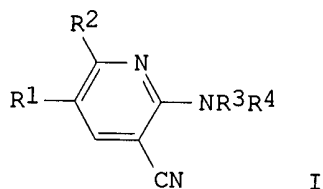
RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 131695-27-7 CAPLUS

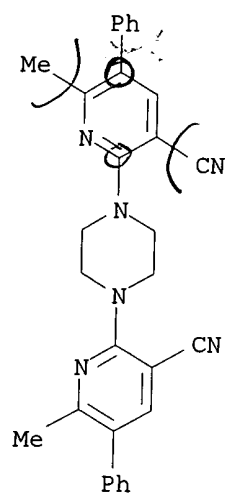
CN 3,5-Pyridinedicarbonitrile, 2,2'-[(ethoxymethylene)diimino]bis[6-methoxy-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



~~LT9~~ ANSWER 11 OF 21 CAPLUS COPYRIGHT 2002 ACS
~~AN~~ 1990:490939 CAPLUS
 DN 113:90939
 TI Potential cardiotonic agents. Part 7: Synthesis and cardiovascular properties of 5-(4-pyridinyl)-, 6-methyl-5-(4-pyridinyl)- and 6-methyl-5-phenyl-substituted 3-cyano-2-aminoalkylaminopyridines
 AU Hagen, V.; Rumler, Andrea; Klauschenz, E.; Hagen, Angela; Heer, Sabine; Faust, G.; Mitzner, R.
 CS Inst. Wirkstofforsch., Akad. Wiss. DDR, Berlin, DDR-1136, Ger. Dem. Rep.
 SO Pharmazie (1990), 45(4), 240-1
 CODEN: PHARAT; ISSN: 0031-7144
 DT Journal
 LA German
 OS CASREACT 113:90939
 GI



AB Twelve title compds. (I, R1 = 4-pyridinyl, Ph; R2 = H, Me; NR3R4 = aminoalkylamino or substituted piperazine) were prepd. by reaction of 2-chloropyridines with the appropriate amine. Some I had greater pos. inotropic activity than amrinone in isolated guinea pig atria, while heart rate decreased or remained unchanged. In anesthetized dogs, some I dose-dependently increased myocardial contractility and, in addn., decreased blood pressure. Introduction of an Me group at position 6 (R2) did not increase the pos. inotropic activity. The compds. most suitable for further investigation were I [R1 = 4-pyridinyl; R2 = H; NR3R4 = NH(CH2)3NEt2] and I (R1 = 4-pyridinyl; R2 = H; NR3R4 = morpholinopropylamino).
 IT **128882-36-0P**
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (prepn. and cardiotonic activity of, structure in relation to)
 RN 128882-36-0 CAPLUS
 CN 3-Pyridinecarbonitrile, 2,2'-(1,4-piperazinediyl)bis[6-methyl-5-phenyl- (9CI) (CA INDEX NAME)



~~129~~ ANSWER 12 OF 21 CAPLUS COPYRIGHT 2002 ACS
 AN 1989:530322 CAPLUS

DN 111:130322

TI Europium chelates with polypyridine and phenanthroline derivatives for fluorescent labels for immunoassays

IN Toner, John Luke

PA Eastman Kodak Co., USA

SO Eur. Pat. Appl., 39 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 288256	A2	19881026	EP 1988-303543	19880420
	EP 288256	A3	19910626		
	R: DE, FR, GB				
	US 4837169	A	19890606	US 1987-40385	19870420
	CA 1292710	A1	19911203	CA 1987-542828	19870723
	JP 01045365	A2	19890217	JP 1988-94703	19880419
	JP 2614893	B2	19970528		
	US 4859777	A	19890822	US 1988-285163	19881216
PRAI	US 1987-40385		19870420		
	US 1981-279398		19810701		
	US 1986-825693		19860203		
	US 1987-7024		19870127		

OS MARPAT 111:130322

GI For diagram(s), see printed CA Issue.

AB Stable fluorescent labels comprise Eu³⁺ and a chelating agent I [R = H, alkyl, alkoxy, alkylthio, alkylamino, (substituted)aryl, aryloxy, heterocycle, enzyme, antigen, antibody; R₁ = R except for aryloxy; R₂ = COO, OH, carbonyliminodiacetic acid, methyleneiminodiacetic acid, hydrazinylideneacetic acid, or the esters or salts of the acids; n = 0-4; m = 0 or 1 when n = 0; II, III, and IV are excluded from the structure] which is a triplet sensitizer having triplet energy > Eu³⁺ and .gtoreq.2 heteroatom-contg. groups which form coordinate complexes with Eu³⁺ and a 3rd heteroatom-contg. group or heteroatom in or appended to the triplet sensitizer. The chelating agents are polypyridines or phenanthrolines. Labeled physiol. active materials such as vitamins, hormones, receptors, etc., and a fluorescence immunoassay, are described. V 0.60 and VI 0.71 g (preps. are described) were refluxed with 5 g NH₄OAc in MeOH 100 mL for 16 h. The soln. was cooled and filtered, and the solid was triturated with hot HCl, filtered, washed with MeOH followed by Et₂O, and dried, to yield VII 0.40 g (53%). A 10-6M soln. of VII and EuCl₃.6H₂O was highly luminescent under long wavelength UV.

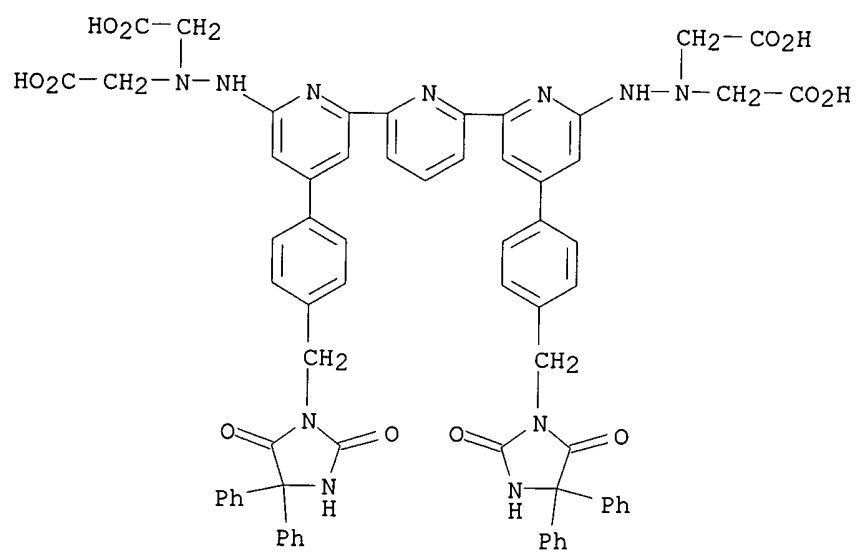
IT **122637-34-7D**, salts, esters, biomol. conjugates

RL: ANST (Analytical study)

(chelating agent, for europium, fluorescence immunoassay in relation to)

RN 122637-34-7 CAPLUS

CN Acetic acid, 2,2',2'',2'''-[[4,4''-bis[4-[(2,5-dioxo-4,4-diphenyl-1-imidazolidinyl)methyl]phenyl][2,2':6',2'''-terpyridine]-6,6''-diyl]di-2-hydrazinyl-1-ylidene]tetrakis- (9CI) (CA INDEX NAME)



~~LI~~ 9 ANSWER 13 OF 21 CAPLUS COPYRIGHT 2002 ACS

~~AN~~ 1989:85465 CAPLUS

~~DN~~ 110:85465

~~TI~~ Electrophotographic photoreceptors with bisazo compound-containing charge-generation layers

~~IN~~ Numa, Tatsuya; Ito, Yuji; Akitsuma, Masatomi; Fujimoto, Masaki

~~PA~~ Nippon Kayaku Co., Ltd., Japan

~~SO~~ Jpn. Kokai Tokkyo Koho, 6 pp.

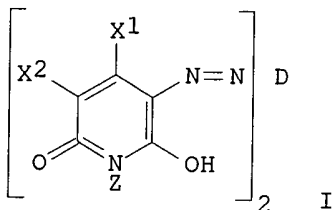
CODEN: JKXXAF

~~DT~~ Patent

~~LA~~ Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 63193153	A2	19880810	JP 1987-24492	19870206
GI					



AB The title photoreceptors contain bisazo compds. of the formula I [D = (un)substituted arylene, divalent heterocyclic group; X1 = (un)substituted alkyl, phenyl; X2 = H, CN, CONH2, CO2R, COR; R = Me, Et; Z = H, alkenyl, cycloalkyl, (un)substituted aryl]. Thus, a dichloroethane soln. of I (D = p-C6H4; X1 = Me; X2 = CN; Z = Bu) and Vylon 200 was applied on an Al-evapd. polyester film to give a charge-generation layer, which was coated with a hydrazone-type charge-transport layer to give an electrophotog. photoreceptor having excellent charging characteristics.

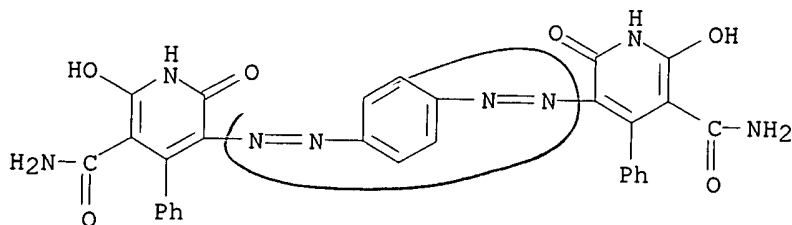
IT 118830-35-6

RL: USES (Uses)

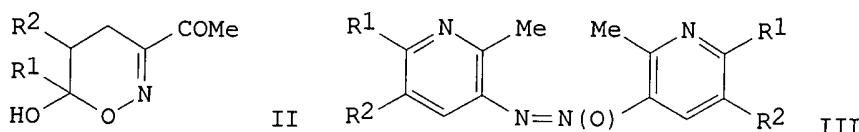
(electrophotog. photoreceptor with charge-generation layer from, with good charging characteristics)

RN 118830-35-6 CAPLUS

CN 3-Pyridinecarboxamide, 5,5'-[1,4-phenylenebis(azo)]bis[1,2-dihydro-6-hydroxy-2-oxo-4-phenyl- (9CI) (CA INDEX NAME)



IN/9 ANSWER 14 OF 21 CAPLUS COPYRIGHT 2002 ACS
 AN 1988:167261 CAPLUS
 DN 108:167261
 TI A synthesis of 3-azoxypyridines by cyclization of hydroxyimino-substituted diketones with ammonia
 AU Gilchrist, Thomas L.; Moxey, John R.; Yagoub, Ahmed K.
 CS Robert Robinson Lab., Univ. Liverpool, Liverpool, L69 3BX, UK
 SO J. Chem. Res., Synop. (1987), (11), 357
 CODEN: JRPSDC; ISSN: 0308-2342
 DT Journal
 LA English
 OS CASREACT 108:167261
 GI



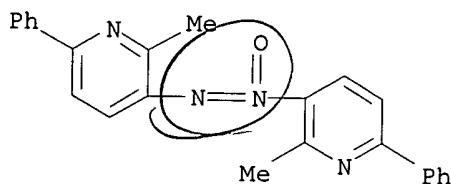
AB Cycloaddn. of nitrosobutenone $\text{CH}_2:\text{C}(\text{COMe})\text{N}:\text{O}$ with alkenes $\text{R}_2\text{CH}:\text{CR}_1\text{X}$ [$\text{R}_1\text{R}_2 = (\text{CH}_2)_n$, $n = 3, 4, 5$; $\text{R}_1 = \text{Ph}$, Me_3C , $\text{R}_2 = \text{H}$; $\text{R}_1 = \text{H}$, $\text{R}_2 = \text{Ph}$; $\text{R}_1 = \text{R}_2 = \text{H}$; $\text{X} = \text{morpholino}$, pyrrolidino , EtO , Me_3SiO] and in situ hydrolysis afforded products which are formulated as open-chain oximes $\text{R}_1\text{COCHR}_2\text{CH}_2\text{C}(\text{NOH})\text{COMe}$ (I) and/or hydroxyoxazines II. Treatment of I/II with aq. NH_3 , in an app. open to the air, gave azoxypyridines III. A mechanism involving oxidn. of intermediate hydroxyaminopyridines is proposed.

IT 113737-96-5P 113737-98-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

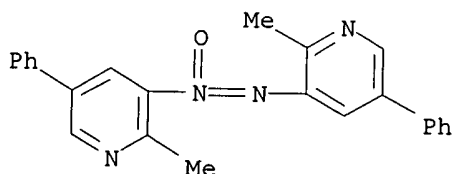
RN 113737-96-5 CAPLUS

CN Pyridine, 3,3'-azoxybis[2-methyl-6-phenyl- (9CI) (CA INDEX NAME)

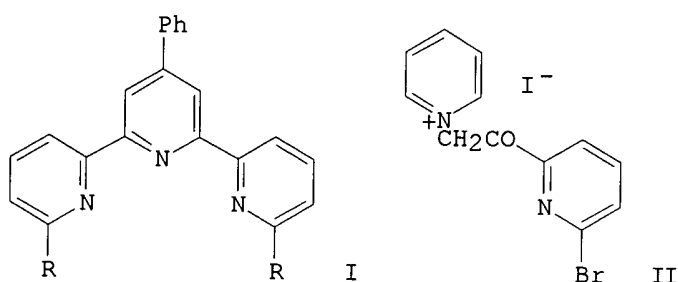


RN 113737-98-7 CAPLUS

CN Pyridine, 3,3'-azoxybis[2-methyl-5-phenyl- (9CI) (CA INDEX NAME)



~~LI~~ 9 ANSWER 15 OF 21 CAPLUS COPYRIGHT 2002 ACS
 AN 1983:107123 CAPLUS
 DN 98:107123
 TI The preparation and coordination chemistry of 2,2':6',2''-terpyridine
 macrocycles - 1
 AU Constable, Edwin C.; Lewis, Jack
 CS Chem. Lab., Univ. Cambridge, Cambridge, CB2 1EW, UK
 SO Polyhedron (1982), 1(3), 303-6
 CODEN: PLYHDE; ISSN: 0277-5387
 DT Journal
 LA English
 GI



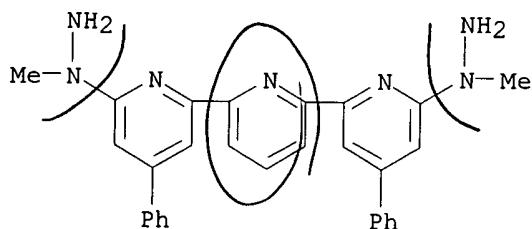
AB Derivs. of 2,2':6',2''-terpyridine were prepd. with the intention of forming macrocycles incorporating the 2,2':6',2''-terpyridyl moiety. Bis(methylhydrazino)phenylterpyridine I (R = MeNNH₂) and a no. of metal complexes of this novel pentadentate ligand were prepd. Thus, Ortoleva-King reaction of 2-acetyl-6-bromopyridine with iodine and pyridine gave pyridinium iodide II. Cyclocondensation of II and 2-bromo-6-cinnamoylpyridine in refluxing HOAc contg. NH₄OAc gave I (R = Br). Reaction of the latter with MeNHNH₂ gave I (R = MeNNH₂) which formed colored complexes with Cr, Mn, Fe, Co, and Ni.

IT **84488-15-3P**

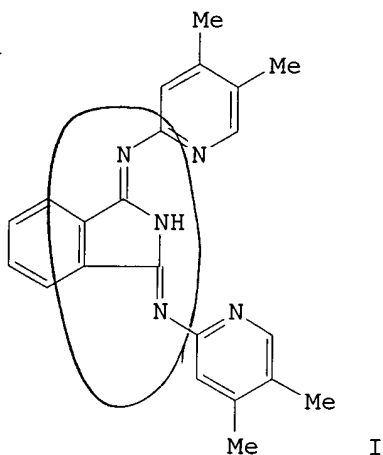
RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 84488-15-3 CAPLUS

CN 2,2':6',2''-Terpyridine, 6,6''-bis(1-methylhydrazino)-4,4''-diphenyl-
 (9CI) (CA INDEX NAME)

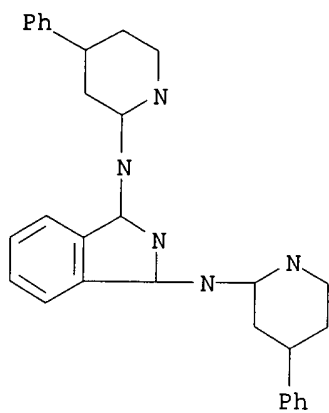


~~LT9~~ ANSWER 16 OF 21 CAPLUS COPYRIGHT 2002 ACS
~~AN~~ 1982:181110 CAPLUS
 DN 96:181110
 TI Metal-chelating 1,3-bis(2-pyridylimino)isoindolines
 AU Siegl, Walter O.
 CS Ford Motor Co., Dearborn, MI, 48121, USA
 SO J. Heterocycl. Chem. (1981), 18(8), 1613-18
 CODEN: JHTCAD; ISSN: 0022-152X
 DT Journal
 LA English
 GI



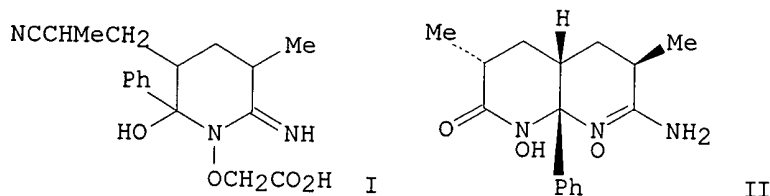
AB A variety of novel chelating 1,3-bis(2-pyridylimino)isoindoline ligands, e.g. I, were prepd. by reaction of phthalonitriles or 1,3-diiminoisoindolines with 2-aminopyridines and characterized including ligands substituted on both the pyridyl and isoindoline ring systems. Noteworthy are the 1st isoindoline ligands with soly. in aq. media. A convenient prepn. of 4-alkoxyphthalonitriles is reported; these compds. are readily obtained from 4-nitrophthalonitrile and are suitable starting materials for alkoxy-substituted ligands.
 IT **81560-17-0P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 81560-17-0 CAPLUS
 CN 1H-Isoindol-3-amine, N-(4-phenyl-2-pyridinyl)-1-[(4-phenyl-2-pyridinyl)imino]- (9CI) (CA INDEX NAME)

09/893,680



*** FRAGMENT DIAGRAM IS INCOMPLETE ***

~~LA~~ 9 ANSWER 17 OF 21 CAPLUS COPYRIGHT 2002 ACS
 AN 1981:460908 CAPLUS
 DN 95:60908
 TI Iminyls. Part 8. Intramolecular addition to nitrile groups
 AU Forrester, Alexander R.; Irikawa, Hajima; Thomson, Ronald H.; Woo, Soo On; King, Trevor J.
 CS Chem. Dep., Univ. Aberdeen, Aberdeen, AB9 2UE, Scot.
 SO J. Chem. Soc., Perkin Trans. 1 (1981), (6), 1712-20
 CODEN: JCPRB4; ISSN: 0300-922X
 DT Journal
 LA English
 GI



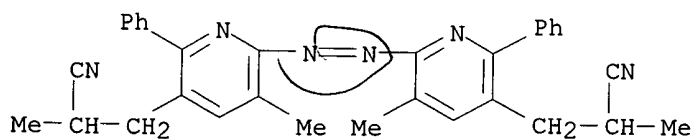
AB Evidence for the radical polymn. of nitrile groups in polyacrylonitrile was sought using model compds. No cycloaddn. of iminyls to nitrile groups was obsd. but nucleophilic addn. occurred readily. E.g., 1,8-(NC)₂C₁₀H₆ reacted with NH₂OH to give naphthalimide dioxime and with BuLi to give azaphenylene derivs. but adamantyl radicals did not attack the nitrile functions. PhCOCH(CH₂CHMeCN)₂ and NH₂OH (NaOAc, aq. EtOH, reflux, 2 h) gave the piperidine I (4.3%) and 2 decahydro-1,8-naphthyridine derivs. rather than the oxime. Reaction of I with BrCH₂CO₂H gave an oxyacetic acid which on persulfate oxidn. gave a cis-trans mixt. of azopyridines. The structure of one of the decahydronaphthyridines (II) was detd. by x-ray anal.

IT **78414-87-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 78414-87-6 CAPLUS

CN 3-Pyridinepropanenitrile, 6,6'-azobis[.alpha.,5-dimethyl-2-phenyl- (9CI)
(CA INDEX NAME)

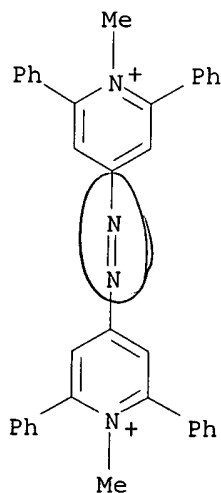


~~119~~ ANSWER 18 OF 21 CAPLUS COPYRIGHT 2002 ACS
~~AN~~ 1975:4099 CAPLUS
 DN 82:4099
 TI Two-step redox systems. XIV. Phenylogs and diazavinylogs of bipyrylium, bithiopyrylium, and bipyridylium salts
 AU Huenig, Siegfried; Ruider, Guenther
 CS Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, Ger.
 SO Justus Liebig's Ann. Chem. (1974), (9), 1415-22
 CODEN: JLACBF
 DT Journal
 LA German
 GI For diagram(s), see printed CA Issue.
 AB The pyrylium salt I ($X = O^+$, $Z = p$ -phenylene, $X^- = BF_4^-$), prepd. according to K. Dimroth and Ch. Reichardt (1969), was converted by treatment with NH_3 and subsequent methylation ($Me_3O^+ BF_4^-$) into .apprx.100% I ($X^+ = N+Me$), whereas the common conversion into $X^+ = S^+$ by Na_2S failed. Reaction of the methylthio compds. II ($X^+ = N+Me$ or S^+) with N_2H_4 in EtOH and DMF gave III ($X^+ = N+Me$ and S^+ , resp.), whereas II ($X^+ = O^+$) reacted likewise only in the presence of AcONa buffer and anhyd. EtOH to give only 17% III ($X^+ = O^+$).
 IT **54787-29-0P 54787-30-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 54787-29-0 CAPLUS
 CN Pyridinium, 4,4'-azobis[1-methyl-2,6-diphenyl-, bis[tetrafluoroborate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 54787-28-9

CMF C36 H30 N4



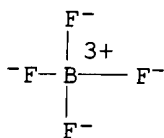
CM 2

CRN 14874-70-5

CMF B F4

CCI CCS

09/893,680

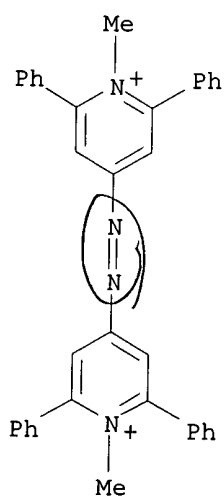


RN 54787-30-3 CAPLUS
CN Pyridinium, 4,4'-azobis[1-methyl-2,6-diphenyl-, diperchlorate (9CI) (CA
INDEX NAME)

CM 1

CRN 54787-28-9

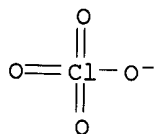
CMF C36 H30 N4



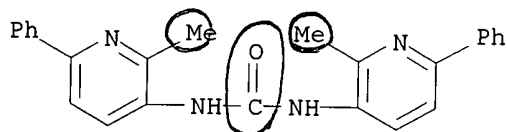
CM 2

CRN 14797-73-0

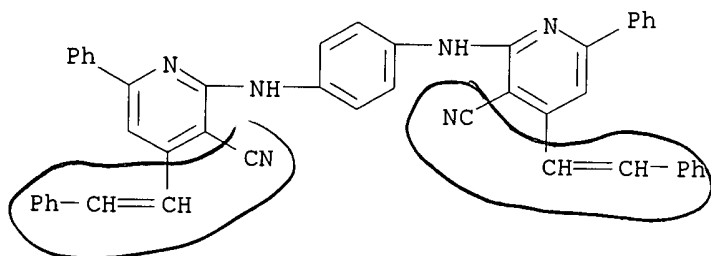
CMF Cl O4



~~L10~~ ANSWER 19 OF 21 CAPLUS COPYRIGHT 2002 ACS
~~AN~~ 1974:108440 CAPLUS
 DN 80:108440
 TI Pyrazolopyridines. III. Preparation and reactions of
 pyrazolo[4,3-b]pyridines
 AU Foster, Hylton E.; Hurst, Jim
 CS Sch. Pharm., Sunderland Polytech., Sunderland, Engl.
 SO J. Chem. Soc., Perkin Trans. 1 (1973), (23), 2901-7
 CODEN: JCPRB4
 DT Journal
 LA English
 GI For diagram(s), see printed CA Issue.
 AB Nitrosation of 3-acetamido-2-methylpyridines with NOCl followed by
 refluxing in C6H6 gave 1-acetyl-1H-pyrazolo[4,3-b]pyridines which were
 deacetylated by HCl. E.g. 3-acetamido-2-methyl-6-phenylpyridine gave 86%
 pyrazolopyridine (I; R = Ph, R1 = Ac) which gave 85% I (R = Ph, R1 = H).
 1- and 2-Acyl derivs. of I (R = Me, R1 = H) (II) were prepd. Bromination
 and nitration of II gave the corresponding 3-bromo and 3-nitro derivs.
 Similarly 1H-pyrazolo[4,3-b]pyridin-5(4H)-one gave 3-bromo, 3,6-dibromo,
 and 3,6-dinitro derivs.
 IT **52090-59-2P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 52090-59-2 CAPLUS
 CN Urea, N,N'-bis(2-methyl-6-phenyl-3-pyridinyl)- (9CI) (CA INDEX NAME)



~~119~~ ANSWER 20 OF 21 CAPLUS COPYRIGHT 2002 ACS
~~AN~~ 1974:82586 CAPLUS
~~DN~~ 80:82586
 TI Some reactions with 1,2-dihydro-2-oxo-6-phenyl-4-styrylnicotinonitrile
 AU Sammour, A.; Raouf, A.; Elkasaby, M.; Hassan, M.
 CS Fac. Sci., Ain Shams Univ., Cairo, UAR
 SO J. Prakt. Chem. (1973), 315(6), 1175-82
 CODEN: JPCEAO
 DT Journal
 LA English
 GI For diagram(s), see printed CA Issue.
 AB The title nicotinonitrile I (R = OH) obtained from Ph(CH:CH)2COPh and NCCH2CO2Et reacted with R1Y (Y = Cl, Br, or iodine), with POCl3, and with R2MgY to give the ethers I (R = OR1; R1 = Me, Et, PhCH2, CH2CH2OH, or CH2CO2Et) (II), the chloride I (R = Cl) (III), and the ketones IV (R = OH; R2 = Me, cyclohexyl, 1-C10H7, Ph, or 2-MeOC6H4), resp. Amination of III gave the amines I (R = NHR3, R3 = Bu, PhCH2, 4-MeOC6H4, PhNH, or HO2CCH2). II (R1 = Me or Et) reacted with R2MgY to give IV (R = OMe or OEt; R2 = Me or Ph). Reaction of IV [R2 = Me (V) or Ph] with NH2OH.HCl in AcOH gave the isoxazolopyridines VI. Reaction of V with R4CHO (Claisen-Schmidt condensation) gave the cinnamoyl derivs. IV [R = OH, R2 = CH:CHR4; R4 = Ph, 4-ClC6H4, or 3,4-(OCH2O)C6H3], the 2 latter of which reacted with PhNHNH2 and NH2OH.HCl to give the pyrazolines VII and the isoxazolines VIII, resp.
 IT **51328-87-1P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 51328-87-1 CAPLUS
 CN 3-Pyridinecarbonitrile, 2,2'-(1,4-phenylenediimino)bis[6-phenyl-4-(2-phenylethenyl)- (9CI) (CA INDEX NAME)



~~LV~~9 ANSWER 21 OF 21 CAPLUS COPYRIGHT 2002 ACS
~~AN~~ 1973:505050 CAPLUS
 DN 79:105050
 TI Reaction of 6-amino-2H-thiopyran-2-thiones with amines
 AU Gewald, K.; Buchwalder, M.; Peukert, M.
 CS Sekt. Chem., Tech. Univ. Dresden, Dresden, Ger.
 SO J. Prakt. Chem. (1973), 315(4), 679-89
 CODEN: JPCEAO
 DT Journal
 LA German
 GI For diagram(s), see printed CA Issue.
 AB Reaction of the thiopyranthiones I, R = CN or CO₂Et, R₁ = Ph, R₂ = H, or R₁R₂ = (CH₂)₄ or of it theirs S-methyl derivs. (II, X = iodide or MeSO₄) with R₃NH₂ (R₃ = OH, NH₂, Me, CH₂Ph, or NHPH) yielded the pyridinethiones III. III (R₃ = NH₂) were deaminated and then rearranged in HCO₂H into the corresponding 2-amino-6-thiocyanatopyridines. Aniline reacted with II but not with I to give the imino derivs. IV, which were rearranged, by treating with bases, into III. Reaction of I with R₄R₅NH (NR₄R₅ = morpholino or piperidino) gave the thiones V.
 IT **50706-82-6P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 50706-82-6 CAPLUS
 CN 3-Pyridinecarboxylic acid, 2,2'-dithiobis[6-(4-morpholinyl)-4-phenyl-, diethyl ester (9CI) (CA INDEX NAME)

